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Area laws for thermal free fermions

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Abstract: We provide a rigorous and asymptotically exact expression of the mutual information of translationally invariant free fermionic lattice systems in a Gibbs state. In order to arrive at this result, we introduce a novel framework for computing determinants of Töplitz operators with smooth symbols, and for treating Töplitz matrices with system size dependent entries. The asymptotically exact mutual information for a partition of the one-dimensional lattice satisfies an area law, with a prefactor which we compute explicitly. As examples, we discuss the fermionic XX model in one dimension and free fermionic models on the torus in higher dimensions in detail. Special emphasis is put onto the discussion of the temperature dependence of the mutual information, scaling like the logarithm of the inverse temperature, hence confirming an expression suggested by conformal field theory. We also comment on the applicability of the formalism to treat open systems driven by quantum noise. In the appendix, we derive useful bounds to the mutual information in terms of purities. Finally, we provide a detailed error analysis for finite system sizes. This analysis is valuable in its own right for the abstract theory of Töplitz determinants.

Contents

1. Introduction

How do the correlations of natural quantum states of many-body systems behave? If "natural" is taken to mean "generic" in the sense of a random pure state drawn from the Haar measure, then the answer to this question is: Subsystems will almost surely be very nearly maximally correlated with their complementary subsystems. However, this is not the situation that one is usually interested in in many-body and condensed-matter physics. Ground states of local Hamiltonians typically exhibit far less entanglement than that suggested by the previous argument. Indeed, there is a large body of evidence [1–33], suggesting that ground states of gapped quantum many-body systems on lattices satisfy an *area law* [1] for the entanglement entropy. In other words, given the pure state of a lattice system, if one distinguishes a certain (connected) region of the lattice, then the von-Neumann (or Renyi) entropy of the reduced state associated with this region does not grow, as one might expect, like the number of degrees of freedom of this region (its "volume"). Instead, it scales like the number of degrees of freedom on the boundary, hence as its "area". Area laws have been shown for all gapped one-dimensional models with local interactions [24, 30, 31]. Extensions to classes of higher-dimensional lattice models have also been obtained [2, 12, 29]. These results and others therefore suggest that ground states of quantum many-body systems are much less entangled than they could be. These measures of entanglement – refined quantities revealing much more detailed information about the structure of correlations than more conventional correlation functions – in a way inherit the decay of correlations. This deep insight is also at the basis of classical efficient simulations of quantum many-body systems: The formulation and analysis of many-body systems in terms of matrix-product and other tensor network states have put this intuition on a solid theoretical footing [1, 34, 35]. In numerical simulations of many-body systems, the importance of such approximations can hardly be overestimated. As a consequence, the last decade has seen an enormous amount of interest in the study of entanglement in quantum many-body systems in the condensed

matter context and in issues of numerical simulation [1, 34–36], entanglement spectra [36–41], and their relationship to quantifiers of topological order [38–41].

Can this analysis be extended to thermal states? A moment of thought reveals that the entanglement entropy should in fact satisfy a volume law for thermal states. However, it turns out that the entanglement entropy is not the right quantity to grasp the correlations of a mixed quantum state. There exist many such measures, but the most natural and the most frequently adopted one is the *mutual information*. For a subset A of sites of the lattice and its complement B, it is defined as

$$I(A:B) = S(\rho_A) + S(\rho_B) - S(\rho), \tag{1}$$

where ρ_A and ρ_B are the reduced states of ρ with respect to A and B, respectively. For pure states, the mutual information reduces to twice the entanglement entropy. One might then hope that this quantity fulfills an area law for thermal states of local hamiltonians on a lattice. This turns out to be true in fact for any fixed temperature [42, 43]. Specifically, for the Gibbs states of a Hamiltonians with local interactions on a lattice, and with bounded operator norm $\|h\|$, one finds that

$$I(A:B) \leq 2\beta\|h\| \; |\partial A|, \tag{2}$$

where ∂A denotes the boundary area of the region labelled A. This statement is in fact surprisingly simple to prove. It following rather directly from the extremality of Gibbs states with respect to the free energy.

The strength of this result - that it is completely general - also constitutes its weakness; Eq. (2) does not say anything about the correlation behaviour of thermal states of specific models. Given that the bound is linearly divergent in the inverse temperature, the law becomes less and less tight in the limit of small temperatures. In particular, at zero temperature, we know that there can be logarithmic corrections to the area law for critical systems. Hence, it would be desirable to have bounds which depend more explicitly on the properties of the system at hand. What is more, asymptotically exact results for important classes of “laboratory” models seem important.

In this work, we present asymptotically exact results for important classes of “laboratory” models. We introduce a framework capable of rigorously computing the mutual information in free fermionic lattice models. This framework is based on new approximation techniques as well as on proof tools for dealing with Töplitz matrices with smooth symbols. We separate the presentation in a discussion of the one-dimensional case and one of the higher-dimensional situation of a cubic lattice with the topology of a torus. We find rigorous area laws for the mutual information that are meaningful in the limit of small temperatures, and converge to the known results for the entanglement entropy for ground states [10, 26]. This feature is even present in higher-dimensional fermionic lattice models [15, 21–23, 25]. For low temperatures, we find a logarithmic divergence of the mutual information in the inverse temperature, in fact confirming predictions of conformal field theory. This scaling suggests that in order to detect criticality, extremely low temperatures are needed. This is an exponential improvement in the inverse temperature to the above bound.

Mathematically, we discuss new methods of approximation, allowing to use Töplitz matrix techniques to studying arbitrary subsystems of translationally invariant fermionic models. What is more, we introduce a novel second order Szegö theorem, simplifying Widom’s formula for smooth symbols. This approach allows to use the trace formula without encountering an infinite sum leading to arbitrarily highly oscillatory terms.

Hence, apart from the application in the study of quantum many-body physics, we expect our results to be a highly useful tool in the abstract theory of Töplitz determinants. The paper is structured as follows:

- In Section 2, we introduce Renyi entropy mutual informations for free fermionic models, discuss fermionic covariance matrices and present new, easily computable and practical upper and lower bounds to mutual informations.
- In Section 3, we go on to formulate the problem, and we provide a synopsis of the mathematical argument. A general proof strategy for computing the mutual information is also provided.
- Section 4.1 contains the main theorem – the asymptotically exact expression for the mutual information – and the core of the proof. Since the argument is general enough to capture expressions deriving from all Renyi entropies, the complete knowledge of the spectrum of reduced states is also obtained in this fashion. This section reports also the main technical progress when it comes to dealing with Töplitz matrices with smooth symbols.
- Section 5 is dedicated to a thorough discussion of the temperature dependence of the area law, with an emphasis on the the very low temperatures behavior.
- We then turn to higher-dimensional free fermionic models on the torus in Section 6, which we can treat with similar methods.
- Finally, we present an outlook in Section 7, comparing the findings with predictions of conformal field theory, and discussing implications to the study of entanglement spectra [36–41]. We also consider the implications for noise-driven, open fermionic quantum many-body systems, as have recently been discussed also in the context of open Majorana wires and notions of noise-driven criticality [44–48].

2. Free fermionic models

In this work, we focus on isotropic translationally invariant fermionic models. For now, we assume the most general form for the couplings. Later, we will concentrate on the fermionic variant of the XX spin model (under the Jordan-Wigner transformation), which is a particularly important special case. In this section, we introduce the class of models discussed here.

2.1. Hamiltonians. We consider free fermionic models on cubic lattices $(\mathbb{Z}_N)^D$ for some even $N \in \mathbb{N}$ as N becomes large. Bi-sected geometries on the torus can be related to the situation of having $D = 1$. For simplicity of notation, but without loss of generality, we will therefore present this one-dimensional case in the main part of this work, while discussing the higher-dimensional situation in Section 6. The Hamiltonian takes the general form

$$H := \sum_{i,j \in \mathbb{Z}_N} f_j^\dagger V_{j,k} f_k, \tag{3}$$

with $V = V^T \in \mathbb{R}^{N \times N}$ being a circulant matrix, referred to as the *Hamiltonian matrix*. We assume the coupling to be an specified, finite-ranged interaction of arbitrary interaction length $r \in \mathbb{N}$. The couplings are defined by a sequence of numbers $(v_k)_{k\in\mathbb{N}}$ with the property that $v_k = 0$ for $k > r$. Then take

$$d_j := v_{|j+1|},\ j = -N/2 + 1, \ldots, N/2, \tag{4}$$

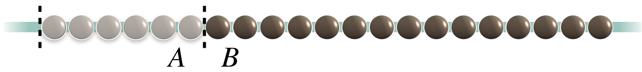

Fig. 1. Geometry of the considered situation for one-dimensional system, consisting of N degrees of freedom, coupled with a local Hamiltonian equipped with periodic boundary conditions. The distinguished region embodying sites $\{0, \ldots, L-1\}$ is referred to as A, its complement is called B.

having a natural reflection symmetry, $d_{-k \bmod N} = d_k$, and consider the Hamiltonian matrix with entries

$$V_{i,j} = d_{(i-j) \bmod N} \tag{5}$$

for $i, j \in \mathbb{Z}_N$. This situation is depicted in Fig. 1. The most important special case is constituted by the fermionic variant of the *XX model*, which is originally a model for spin-$1/2$ systems. Here, we directly consider its fermionic instance, by virtue of the Jordan Wigner transformation. In this language,

$$v_1 = a,\ v_2 = b,\ v_k = 0 \tag{6}$$

for $a, b \in \mathbb{R}$ and $2 < k \in \mathbb{N}$, so that V is a circulant matrix with a on the main diagonal and b on the first off-diagonal. All these models are integrable and exactly solvable. Thermal states are defined entirely by the collection of second moments of fermionic operators. The arbitrary finite range of interactions has in the main text been chosen for simplicity of notation only, and exponentially decaying interactions can easily be accommodated as well. A generalisation to exponentially decaying interactions is possible. Since V is circulant, we find the spectrum $\{\varepsilon_k\}$ of V to be

$$\frac{1}{N} \sum_{k \in \mathbb{Z}_N} \varepsilon_k \mathrm{e}^{2\pi \mathrm{i} k/N} = d_k. \tag{7}$$

For the well-studied fermionic variant of the XX model, see Eq. (6), one gets the familiar expression

$$\varepsilon_k = a + 2b \cos\left(\frac{2\pi \mathrm{i} k}{N}\right). \tag{8}$$

2.2. Majorana fermions and covariance matrices. It is convenient to define fermionic *covariance matrices* in terms of *Majorana fermions*:

$$r_i := \frac{f_i + f_i^\dagger}{\sqrt{2}},\ r_{i+N} := \frac{f_i - f_i^\dagger}{\sqrt{2}\mathrm{i}},\ i = 0, \ldots, N-1, \tag{9}$$

similar to the canonical coordinates for bosonic operators. These Majorana fermions are Hermitian, traceless, and form a Clifford algebra. We are interested in thermal states of the quadratic Hamiltonians, which are particular instances of (quasi)-free or Gaussian fermionic states. Such states are completely specified by their fermionic covariance matrix [25, 44, 49, 50] $\gamma \in \mathbb{R}^{2N \times 2N}$ with entries

$$\gamma_{i,j} = \mathrm{i}\,\mathrm{tr}\left(\rho[r_i, r_j]\right), \tag{10}$$

$i, j = 0, \ldots, 2N-1$, where the brackets denote the commutator. γ is always antisymmetric,

$$\gamma = -\gamma^T, \tag{11}$$

and satisfies $-\gamma^2 \leq \mathbb{1}$.

2.3. Covariance matrices of Gibbs states and their reductions. Matrix functions of the covariance matrix can be computed exactly. This is the case because any covariance matrix is unitarily equivalent to a direct sum of 2×2 covariance matrices, reflecting a situation of entirely uncoupled fermionic modes. This is the fermionic analogue of what is often called the Williamson normal form in the bosonic setting. As a consequence, one can identify an explicit expression for the covariance matrix of *Gibbs states*

$$\rho = \frac{\mathrm{e}^{-\beta H}}{\mathrm{tr}(\mathrm{e}^{-\beta H})} \tag{12}$$

at inverse temperature $\beta > 0$. The covariance matrix $\gamma \in \mathbb{R}^{2N \times 2N}$ of ρ is given by

$$\gamma = \begin{pmatrix} 0 & f(h) \\ -f(h) & 0 \end{pmatrix}, \tag{13}$$

where $f : \mathbb{R} \to \mathbb{R}$ is defined as

$$f(x) := 2\frac{\mathrm{e}^{-\beta x}}{\mathrm{e}^{-\beta x} + 1} - 1 = -\tanh\left(\frac{\beta x}{2}\right). \tag{14}$$

We suppress the temperature dependence here: Throughout this work, we will be concerned with Gibbs states with respect to some β. We allow for arbitrary temperatures and will also later consider the asymptotic limits $\beta \to \infty$ and $\beta \to 0$.

Reduced states of Gaussian states are always Gaussian (as can be seen most easily by considering their Grassman representation; compare Ref. [49]). The covariance matrix of a reduced state is the appropriate principle sub-matrix of the full covariance matrix. Applied to Gibbs states, we find that the reduced state of a subset $A = \{0, \dots, L-1\} \subset \{0, \dots, N-1\}$ is a Gaussian state with covariance matrix

$$\gamma|_A = \begin{pmatrix} 0 & f(h)|_A \\ -f(h)|_A & 0 \end{pmatrix}, \tag{15}$$

where $.|_A$ denotes the principal sub-matrix associated with the degrees of freedom of subsystem A.

2.4. Töplitz matrices. Töplitz matrices [51–53] may be viewed as principal sub-matrices of infinite circulant matrices. Such matrices will play a crucial role in this work. Throughout, we will encounter families of *Töplitz matrices* $T_n \in \mathbb{R}^{n \times n}$, whose entries are given by

$$(T_n)_{i,j} = t_{i-j} \tag{16}$$

for some sequence of reals $(t_k)_{k \in \mathbb{Z}}$. Colloquially speaking, such Töplitz matrices largely resemble circulant matrices, with the "upper right and lower left corners" deviating from a strict circulant matrix. In fact, most of the theory on Töplitz matrices (Töplitz determinants) is in one way or the other concerned with the error made when replacing a Töplitz matrix by a circulant matrix of the same dimension. Later on we will consider sub-matrices of large finite circulant matrices. It is clear that this sequence of Töplitz matrices is defined entirely in terms of the sequence of numbers $(t_k)_{k \in \mathbb{N}}$. This sequence

of numbers - and hence the sequence of Töplitz matrices - is most conveniently represented in therms of its symbol, defined as the inverse Fourier transform on the torus $\mathbb{T} := \{x \in \mathbb{C} : |x| = 1\}$ of $(t_k)_{k\in\mathbb{Z}}$; i.e. the *symbol* $t \in L_\infty(\mathbb{T})$[1] is defined as

$$t_k = \frac{1}{2\pi}\int_0^{2\pi} d\theta t(\mathrm{e}^{\mathrm{i}\theta})\mathrm{e}^{-\mathrm{i}k\theta}. \tag{17}$$

The decay of the Fourier coefficients is directly related to the regularity properties of the symbol. The summability of the coefficients (i.e., $\sum_{k\in\mathbb{Z}} |t_k| < \infty$) is sufficient to ensure $t \in L_\infty(\mathbb{T})$. The relationship between the decaying behaviour of the Fourier coefficients and the regularity of the symbol will be used very frequently. In fact, given our assumptions on the interaction parameters, much better regularity results can be derived as we will show and use later on. Mathematically, $t \in L_\infty(\mathbb{T})$ is equivalent to the requirement that the associated Töplitz operator generates a continuous linear operator on $l^2(\mathbb{N})$. Furthermore, note that all spectra can be expressed entirely in terms of the symbol.

The starting point of our analysis is the following observation: covariance matrices of subsystems of thermal states of translationally invariant fermionic models are well approximated by Töplitz matrices. Since the Hamiltonian matrix V in Eq. (3) is circulant, the covariance matrix γ of a Gibbs state ρ is, for any $\beta > 0$, circulant as well. That is to say,

$$\gamma_{i,j} = l_{i-j \bmod N}, \tag{18}$$

for some real sequence $(l_k)_{k\in\mathbb{Z}}$, suppressing the temperature dependence. Indeed, submatrices $\gamma|_A$ for a region $A = \{0, \ldots, L-1\}$ of the full covariance matrix γ (of the large but finite system) can be well approximated by the Töplitz matrix $\gamma_L \in \mathbb{R}^{L\times L}$ for large N (see Section 4.2). Th family of Töplitz matrices γ_L can be expressed in terms of the symbol

$$\lambda = f \circ \varepsilon \tag{19}$$

where $\varepsilon \in L_\infty(\mathbb{T})$ is defined as

$$\varepsilon(x) = \sum_{k\in\mathbb{Z}} d_k x^k. \tag{20}$$

Again, via the inverse Fourier transform on the torus, one recovers

$$d_k = \frac{1}{2\pi}\int_0^{2\pi} d\theta \varepsilon(\mathrm{e}^{\mathrm{i}\theta})\mathrm{e}^{-\mathrm{i}k\theta}, \tag{21}$$

where $(d_k)_{k\in\mathbb{Z}}$ is just the sequence of numbers that govern the coupling in the Hamiltonian matrix in Eq. (3).

[1] As usual, $L_p(\mathbb{T})$ denotes the set of equivalence classes of $p-$integrable functions up to functions that vanish almost everywhere on $\mathbb{T}$, with $p = \infty$ denoting the equivalence classes with finite essential supremum.

2.5. Entropies of fermionic Gaussian states. Given that the states we consider are completely described by their covariance matrices, we are able to explicitly compute their Renyi, and specifically von-Neumann, entropies explicitly and efficiently. In particular, we consider covariance matrices of the form

$$\gamma = \begin{pmatrix} 0 & X \\ -X & 0 \end{pmatrix} \tag{22}$$

where $X = X^T \in \mathbb{R}^{n\times n}$. For fermionic Gaussian states ρ of n modes with a covariance matrix of this form one finds

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \log_2 \operatorname{tr}(\rho^\alpha) = \operatorname{tr}(s_\alpha(X)), \tag{23}$$

where the function $s_\alpha : [-1,1] \to [0,1]$ is defined as

$$s_\alpha(x) := \frac{1}{1-\alpha} \log_2 \left(\left(\frac{1+x}{2}\right)^\alpha + \left(\frac{1-x}{2}\right)^\alpha \right). \tag{24}$$

Taking the limit as $\alpha \to 1$, one recovers the von-Neumann entropy,

$$S(\rho) = \operatorname{tr}(s(X)) \tag{25}$$

with $s : [-1,1] \to [0,1]$ being

$$s(x) = -\frac{1+x}{2} \log_2 \left(\frac{1+x}{2}\right) - \frac{1-x}{2} \log_2 \left(\frac{1-x}{2}\right). \tag{26}$$

These expressions will be central for our analysis.

3. Statement of the problem

3.1. Computing mutual informations. We will now turn to the main object of our study, the *mutual information*; a measure of the correlations between two non-overlapping subsystems. We will consider a one-dimensional lattice with N lattice sites and let $A = \{0, \ldots, L-1\}$ constitute one part and $B = \{L, \ldots, N-1\}$ its complement. The quantum mutual information between A and B is defined as

$$I(A : B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \tag{27}$$

where again, ρ is a state on the entire system, ρ_A (ρ_B) is obtained by tracing out subsystem A (B). The mutual information naturally captures all correlations, quantum as well as classical, between A and B. It is a meaningful measure of correlation for mixed states, including finite temperature thermal states as a special case. For zero temperature, it reduces to (twice the) *entanglement entropy*. Similarly, expressions of the kind

$$I_\alpha(A : B) = S_\alpha(\rho_A) + S_\alpha(\rho_B) - S_\alpha(\rho) \tag{28}$$

for an $\alpha > 0$ different from 1 are well defined mutual Renyi entropies. We will identify novel formulae for the asymptotic behavior of the mutual information for Gibbs states of isotopic translationally invariant free-fermionic models, and present bounds that allow to study the limit of large β analytically. The formulae given will be exact in the asymptotic limit of large N.

3.2. Structure of the argument for one-dimensional systems. A number of steps will be necessary in order to arrive at an asymptotically exact expression of the mutual information. To start with, we need to have a handle on how to make the intuition rigorous that we can compute $S_\alpha(\rho_A)$ (and $S_\alpha(\rho_B)$) as if it was the reduced state of an infinite system. The result has to fit then with the expression for $S_\alpha(\rho)$ for the entire system, in a way that only the boundary terms remain. The turns out to be a delicate a faire, and requires very different tools than the pure state analysis, where the asymptotically exact entanglement entropy is obtained using the Fisher-Hartwig formalism [10]. In the case of thermal states, the so-called "double scaling limit" makes sense, where A is taken as a constant fraction of the total system size, and the total system is taken to infinity.

We aim at computing an asymptotically exact approximation of the entropy of a subsystem

$$S_\alpha(\rho_A) = \operatorname{tr}\left(s_\alpha\left(X|_A\right)\right), \tag{29}$$

where $X \in \mathbb{R}^{N\times N}$ is given by

$$X_{k,l} := x_{k-l} := \frac{1}{N}\sum_{j=0}^{N-1} \lambda(\mathrm{e}^{2\pi \mathrm{i} j/N})\mathrm{e}^{-2\pi \mathrm{i} j(k-l)/N}. \tag{30}$$

The proof strategy is as follows:

- We perform a continuum limit on the full system

$$X_{k,l}^{(N)} \to X_{k,l}^{(\infty)} := x_{k-l}^{(\infty)} := \frac{1}{2\pi}\int_0^{2\pi} \lambda(\mathrm{e}^{\mathrm{i}\phi})\mathrm{e}^{-\mathrm{i}(k-l)\phi}d\phi, \tag{31}$$

  and show that the entropy of a subsystem can be computed with an exponentially small error in N.
- When computing entropies of sub-matrices $S_\alpha(\rho_A)$, we can in this continuum limit invoke the theory of Töplitz matrices, even though the entries of the Töplitz matrices actually depend (very slightly) on the system size. We can therefore consider families of Töplitz matrices with symbol

$$\lambda = f \circ \varepsilon. \tag{32}$$

  The same approach is feasible for $S_\alpha(\rho_B)$.
- We apply trace formulae of Töplitz matrices with smooth symbols. This will allow us to compute an asymptotically exact expression of the entropy of both subsystems.
- We find an expression for the entropy of the total system $S_\alpha(\rho)$, asymptotically exact in the limit of large N.
- The expression for the mutual information found in this way will contain an infinite sum, reflecting the infinite number of modes in momentum space in the asymptotic limit. As such, this formula can not be evaluated. This obstacle we will overcome by a new technique that we introduce, making use of the theory of highly oscillatory integrands. This technique is expected to be of significant interest also outside this context, when analysing properties of families of Töplitz matrices with smooth symbols.

The combination of these steps will allow us to provide an asymptotically exact rigorous and computable expression for the mutual information.

4. Main result

In this section, we will state the main results for one-dimensional systems. We will first present the main theorem and then continue with the proof of the theorem. This will require a number of techniques that we will lay out in later subsection s. The specifically important case of the XX model, the temperature dependence as well as the situation of free fermions on the torus will be discussed in later sections.

In accordance with the analysis of the previous section, we will evaluate the mutual information by analyzing the determinants of the covariance matrices, as the system is taken to the thermodynamics limit. Covariance matrices of free fermionic systems in one dimension are Töplitz matrices, so we are free to use the tools available from the theory of Töplitz determinants. In particular, it is well known that Töplitz determinants behave in a very regular manner as the dimension of the matrices are taken to infinity. In the case when the symbol is continuous, Szegö's strong limit theorem [57] gives the precise scaling of the determinant with the dimension of the Töplitz matrix. When the symbol has discontinuities, then it is necessary to use the Fisher Hartwig formula in order to obtain accurate asymptotics. As we will be dealing with thermal states, the symbols will always be continuous, even though a discontinuous symbol reflecting the Fermi surface can be arbitrarily well approximated for low temperatures. This creates a quite intriguing situation: We can "approximate" the situation covered by the Fisher-Hartwig theorem arbitrarily well with smooth symbols, and can hence "interpolate" between these situations. As mentioned before, the methods developed here are expected to be useful also outside the context of quantum many-body systems.

4.1. Main theorem for one-dimensional systems. We consider the mutual information in the large N limit, where

$$|A| = L = \theta(N), \ |B| = \theta(N), \tag{33}$$

meaning that both subsystems grow linearly in N. Specifically we assume

$$A = \{0, 1, \ldots, \lceil qN \rceil - 1\} \tag{34}$$

and

$$B = \{\lceil qN \rceil, \lceil qN \rceil + 1, \ldots, N-1\}. \tag{35}$$

The main result for one-dimensional bi-sected systems can be stated as follows.

Theorem 1 (Asymptotically exact expression for the mutual information). *For any inverse temperature $\beta > 0$, and for any $\alpha \in [0, \infty)$, the mutual information is given by the, in N asymptotically exact, expression*

$$I_\alpha(A:B) = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} d\phi \int_{-\pi}^{\pi} d\theta \frac{s_\alpha(\lambda(\mathrm{e}^{\mathrm{i}\theta})) - s_\alpha(\lambda(\mathrm{e}^{\mathrm{i}\phi}))}{\lambda(\mathrm{e}^{\mathrm{i}\theta}) - \lambda(\mathrm{e}^{\mathrm{i}\phi})} \frac{\lambda'(\phi) - \lambda'(\theta)}{\tan((\phi-\theta)/2)} + o(1). \tag{36}$$

Here, the temperature dependence is only implicit in $\lambda = f \circ \varepsilon$ (since f depends on β), while λ' denotes the derivative of λ, which has to be understood in the following way,

$$\lambda'(\theta) := \frac{d}{d\theta} \lambda(\mathrm{e}^{\mathrm{i}\theta}). \tag{37}$$

This is an asymptotically exact and simply evaluated expression. The most important instance is the one for the von-Neumann mutual information.

Proposition 1 (Mutual information as an infinite sum). *For any inverse temperature $\beta > 0$, and for any $\alpha \in [0, \infty)$, the mutual information is given by the, in N asymptotically exact, expression*

$$I_\alpha(A:B) = \frac{1}{2\pi^2} \sum_{k=1}^{\infty} \int_{-\pi}^{\pi} d\phi \int_{-\pi}^{\pi} d\theta \frac{s_\alpha\left(\lambda(\mathrm{e}^{\mathrm{i}\theta})\right) - s_\alpha\left(\lambda(\mathrm{e}^{\mathrm{i}\phi})\right)}{\lambda(\mathrm{e}^{\mathrm{i}\theta}) - \lambda(\mathrm{e}^{\mathrm{i}\phi})} \times \sin\left(k(\theta - \phi)\right)\left(\lambda'(\phi) - \lambda'(\theta)\right) + o(1). \tag{38}$$

The proof of this statement will require some preparation.

4.2. Approximation statements. In this subsection, we collect approximation statements that are being used in the proof of Theorem 1. We have a more detailed look at the expression

$$X_{k,l}^{(N)} = x_{k-l}^{(N)} = \frac{1}{N} \sum_{j=0}^{N-1} \lambda(\mathrm{e}^{2\pi \mathrm{i} j/N}) \mathrm{e}^{-2\pi \mathrm{i} j(k-l)/N} \tag{39}$$

as well as at

$$X_{k,l} = x_{k-l} = \frac{1}{2\pi} \int_0^{2\pi} \lambda(\mathrm{e}^{\mathrm{i}\phi}) \mathrm{e}^{-\mathrm{i}(k-l)\phi} d\phi, \tag{40}$$

where the entries of the finite Töplitz matrices are always assumed mod N. We know that

$$S_\alpha(\rho_A) = \mathrm{tr}(s_\alpha(X^{(N)}|_A)), \;\; S_\alpha(\rho_B) = \mathrm{tr}(s_\alpha(X^{(N)}|_B)). \tag{41}$$

Expression Eq. (31) is the continuum limit of Eq. (30). Therefore, from a physical perspective, it seems justified to replace $x_{k-l}^{(N)}$ by its infinite-system counterpart $x_{k-l}^{(\infty)}$ in the calculation of the entropy if the system is large enough. In the next lemma we will show that for any fixed temperature, the error made by this replacement decays exponentially in N.

Lemma 1 (Approximation of entropies of subsystems). *For A, B given by Eq. (34) and Eq. (35) the errors*

$$e_{A,\beta}(N) := |\,\mathrm{tr}(s_\alpha(X^{(N)}|_A)) - \mathrm{tr}(s_\alpha(X|_A))| \tag{42}$$

and

$$e_{B,\beta}(N) := |\,\mathrm{tr}(s_\alpha(X^{(N)}|_B)) - \mathrm{tr}(s_\alpha(X|_B))| \tag{43}$$

are exponentially small in N for fixed $\beta > 0$. More precisely, there exist some N-independent constants $\alpha_{A,\beta}, \alpha_{B,\beta} > 0$, (depending on β, q and the explicit form of the symbol λ), such that

$$\lim_{N\to\infty} \exp(N\alpha_{X,\beta}) e_{k,\beta}(N) = 0 \text{ for } X \in \{A, B\}\,. \tag{44}$$

Proof. The proof for the set B is completely analogous to the proof for the set A, so we will consider the latter subset A only. We will proceed in four steps:

1. We use regularity properties of s_α to bound the total error by the error in the eigenvalues originating from the replacement of $X^{(N)}|_A$ by $X|_A$.
2. We bound the latter by the square norm of the difference of both matrices.
3. We write the square norm as an appropriate sum of $|x_k^{(N)} - x_k|$.

4. Note that $|x_k^{(N)} - x_k|$ is the well-known error of approximating an integral by a sum using the trapezoidal rule.

For technical reasons, it is adventageous to reverse the order. So we start with the last step and consider step three, step two and step one afterwards. The function $\phi \mapsto \lambda(\mathrm{e}^{\mathrm{i}\phi})$ is real-analytic and $2\pi-$periodic with values in some compact subinterval of $(-1, 1)$. By the first part of Lemma 2 there exist some constants $\kappa > 0$ and $M > 0$ such that

$$\lambda\left(\mathrm{e}^{\mathrm{i}\phi}\right) \leq M \text{ for all } \phi \in D, \tag{45}$$

where

$$D := \{x \in \mathbb{C} : |\Im(x)| \leq \kappa\}. \tag{46}$$

This implies

$$\left|\lambda\left(\mathrm{e}^{\mathrm{i}\phi}\right)\mathrm{e}^{\mathrm{i}k\phi}\right| \leq M\mathrm{e}^{|k|\kappa} \tag{47}$$

for all $k \in \mathbb{Z}$. Therefore, by Lemma 2 we get

$$\left|x_k^{(N)} - x_k\right| \leq \frac{2M\mathrm{e}^{|k|a}}{\mathrm{e}^{aN} - 1} \leq \frac{2M\mathrm{e}^{La}}{\mathrm{e}^{aN} - 1} = \frac{2M\mathrm{e}^{\lceil qN\rceil a}}{\mathrm{e}^{aN} - 1}. \tag{48}$$

For the third step note that

$$\left\|X^{(N)}|_A - X|_A\right\|_2^2 = \sum_{j=-(L-1)}^{(L-1)} (L - |j|)\left|x_j^{(N)} - x_j\right|^2, \tag{49}$$

which follows directly from counting the number of entries in both Töplitz matrices. For the second step let $\mu_r^{(A)}$ denote the r-th eigenvalue of X_A and let $\mu_r^{(N,A)}$ denote the r-th eigenvalue of $X_A^{(N)}$. Possibly relabeling these eigenvalues, the Hoffman-Wielandt theorem (Lemma 3) yields

$$\sum_{r=0}^{L-1}\left|\mu_r^{(N,A)} - \mu_r^{(A)}\right|^2 \leq \left\|X^{(N)}|_A - X|_A\right\|_2^2. \tag{50}$$

Finally, note that the Renyi entropy functions s_α are Hölder continuous (see Lemma 4) with some appropriate Hölder exponent $0 < \gamma \leq 1$. In other words, there exists some constant $C > 0$ such that

$$|s_\alpha(x) - s_\alpha(y)| \leq C\,|x - y|^\gamma. \tag{51}$$

This gives the estimate

$$\begin{aligned} e_{A,\beta}(N) &\leq \sum_{r=0}^{L-1}\left|s_\alpha(\mu_r^{(N,L)}) - s_\alpha(\mu_r^{(L)})\right| \\ &\leq C\left(\sum_{r=0}^{L-1}\left|\mu_r^{(N,L)} - \mu_r^{(L)}\right|^\gamma\right) \\ &\leq C\left(\sum_{r=0}^{L-1}\left|\mu_r^{(N,L)} - \mu_r^{(L)}\right|^2\right)^{\gamma/2} L^{1-\gamma/2}, \end{aligned} \tag{52}$$

where we have used Hölder's inequality in the third line. Combining Eq. (52), (50), (49), and (48), the desired result follows for any constant

$$\alpha_{A,\beta} < \gamma\kappa(1-q). \tag{53}$$

Moreover, since γ can be chosen to be 1 for $\alpha > 1$ and arbitrary closed to 1 for the von-Neumann entropy, any rate

$$\alpha_{A,\beta} < \kappa(1-q) \tag{54}$$

will satisfy the required condition for $\alpha \geq 1$. Repeating these steps for subset B yields, for any rate

$$\alpha_{B,\beta} < \gamma\kappa q, \tag{55}$$

the validity of the lemma. $\square$

Lemma 2 (Error estimate [54]). *Let $h : \mathbb{R} \longrightarrow \mathbb{R}$ be real analytical and 2π-periodic. Then there exists a strip $D = \mathbb{R} \times (-\kappa, \kappa) \subset \mathbb{C}$ with $\kappa > 0$ such that h can be extended to a holomorphic and 2π-periodic bounded function $h : D \longrightarrow \mathbb{C}$. The error for the rectangular rule can be estimated by*

$$\left| \frac{1}{2\pi}\int_0^{2\pi} h(x)dx - \frac{1}{n}\sum_{k=1}^{n} h\left(\frac{2\pi k}{n}\right) \right| \leq \frac{4\pi M}{e^{n\kappa}-1}, \tag{56}$$

where M denotes a bound for the holomorphic function h on D.

Note that the constant κ will not depend on n, however it will clearly depend on the function h. It is natural to ask how κ will depend on β if M is kept at a fixed value when we choose h to be the symbol of the covariance matrix of the thermal state of, say, the fermionic instance of the XX model (see Section 5). The answer is that $\kappa \propto \beta^{-1}$ for large β.
To see this fix some $\alpha > 0$ and define

$$M_\alpha := \sup \left\{ \left| \tanh(x) \right| |\Im(x)| \leq \alpha\frac{\pi}{2} \right\} \tag{57}$$

Note that $M_\alpha < \infty$ if and only if $\alpha < 1$ since the hyperbolic tangent has a pole at $\pm\mathrm{i}\frac{\pi}{2}$. Define the set

$$\tilde{D}_\alpha := \left\{ z \in \mathbb{C} \,\middle|\, \left|\Im\left(\beta\left(\frac{a}{2} + b\cos(z)\right)\right)\right| \leq \frac{\alpha\pi}{2} \right\} \tag{58}$$

then obviously $h(z) \leq M_\alpha$ for all $z \in \tilde{D}_\alpha$. From $\Im(\cos(z)) = \sin(\Re(z))\sinh(-\Im(z))$ follows:

$$D_\alpha := \left\{ z \in \mathbb{C} \,\middle|\, |\Im(z)| \leq \operatorname{arsinh}\left(\frac{\alpha\pi}{2b\beta}\right) \right\} \subseteq \tilde{D}_\alpha \tag{59}$$

For fixed $\alpha < 1$ set $\kappa := \operatorname{arsinh}\left(\frac{\alpha\pi}{2b\beta}\right)$ and $D := D_\alpha$. Then h is bounded by the positive real number M_α on D. Moreover for any $\alpha \geq 1$, h is necessarily unbounded on D_α. The asymptopic scaling in β follows from

$$\lim_{\beta\to\infty} \beta \operatorname{arsinh}\left(\frac{\alpha\pi}{2b\beta}\right) = \frac{\alpha\pi}{2b} \tag{60}$$

Lemma 3 (Hoffman and Wielandt [55]). *Let $A, E \in M_n$ be normal matrices and let $(\lambda_1, \lambda_2, \cdots, \lambda_n)$ be the eigenvalues of A in some given order and let $(\mu_1, \mu_2, \cdots, \mu_n)$ be the eigenvalues of $A + E$ in some order. Then there exists a permutation $\sigma \in S_n$ such that*

$$\left(\sum_{i=1}^{n} \left|\mu_{\sigma(i)} - \lambda_i\right|^2\right)^{\frac{1}{2}} \leq \|E\|_2 . \tag{61}$$

Lemma 4 (Hölder continuity of entropy functions). *The (covariance) Renyi entropy functions s_α and the (covariance) von-Neumann entropy function s are Hölder continuous on $[-1,1]$, i.e., there exist $0 < \gamma \leq 1$ and $C > 0$ such that*

$$|s_\alpha(x) - s_\alpha(y)| \leq C\,|x-y|^\gamma \text{ for all } x, y \in [-1,1]. \tag{62}$$

Possible Hölder exponents are

– $0 < \gamma \leq \alpha$ *for* $\alpha < 1$,
– $0 < \lambda < 1$ *for the von-Neumann entropy and*
– $0 < \lambda \leq 1$ *for* $\alpha > 1$.

Proof. To start with, note that the first derivative of s_α (see Eq. (141) in the Appendix), is uniformly bounded in x and y whenever $\alpha > 1$, which proves Hölder continuity with Hölder exponent $\lambda \leq 1$ for $\alpha > 1$. For $0 < \alpha < 1$, there exist constants $C_1, C_2 > 0$ such that

$$|s'_\alpha(x)| \leq \left(C_1 + \frac{C_2}{\alpha}\left((1+x)^{\alpha-1} + (1-x)^{\alpha-1}\right)\right). \tag{63}$$

This yields for any $-1 \leq x < y \leq 1$

$$\begin{aligned} |s_\alpha(x) - s_\alpha(y)| &= \left|\int_x^y s'_\alpha(z)dz\right| \qquad (64)\\ &\leq \int_x^y \left(C_1 + \frac{C_2}{\alpha}\left((1+z)^{\alpha-1} + (1-z)^{\alpha-1}\right)\right)dz \\ &= C_1\,|y-x| + C_2\left(|(1+y)^\alpha - (1+x)^\alpha| + |(1-y)^\alpha - (1-x)^\alpha|\right). \end{aligned}$$

Therefore,

$$\limsup_{x\to y} \frac{|s_\alpha(x) - s_\alpha(y)|}{|y-x|^\alpha} \leq C_2. \tag{65}$$

Hence, for every $x \in [0,1]$, there exists some open neighbourhood $U_x \subseteq [-1,1]$ such that

$$\frac{|s_\alpha(x) - s_\alpha(y)|}{|y-x|^\alpha} \leq 2C_2 \tag{66}$$

for every $y \in U_x$. Then Hölder continuity follows from compactness of $[-1,1]$. This proves the validity of the statement for $\alpha < 1$. For the von-Neumann entropy note that by Eq. (143), s' has logarithmic poles at ± 1. Following the same line of reasoning again yields Hölder continuity of the (covariance) von-Neumann entropy for any Hölder exponent $\lambda < 1$. □

4.3. Relating the mutual information to trace functions of Töplitz matrices. Given that we are interested not in the entropy of a subsystem, but in the mutual information, we will need to consider a second order asymptotic formula for the entropy functionals. This is due to the fact that the bulk contribution of the entropy is cancelled out in the expression for the mutual information, and we are left only with the contribution originating from the boundary. We will therefore require a Szegö's strong limit theorem which contains explicit expressions for the second order contributions. In order to formulate the theorem, we will have to introduce some definitions and notation. It will be necessary to consider sequences of truncations of Töplitz matrices – in our case principal sub-matrices of covariance matrices. We will define the following classes of symbols. The *Wiener algebra*

$$W := \left\{ \mu \in L_\infty(\mathbb{T}) : \sum_{n\in\mathbb{Z}} \left| \frac{1}{2\pi} \int_0^{2\pi} \mu(\mathrm{e}^{\mathrm{i}\theta}) \mathrm{e}^{-\mathrm{i}n\theta} d\theta \right| < \infty \right\}, \tag{67}$$

the *Besov space*

$$B_2^{\frac{1}{2}} := \left\{ \mu \in L_2(\mathbb{T}) : \sum_{n\in\mathbb{Z}} (|n|+1) \left| \frac{1}{2\pi} \int_0^{2\pi} \mu(\mathrm{e}^{\mathrm{i}\theta}) \mathrm{e}^{-\mathrm{i}n\theta} d\theta \right|^2 < \infty \right\}, \tag{68}$$

the *Krein algebra*

$$W \cap B_2^{\frac{1}{2}}, \tag{69}$$

and the space of piecewise continuous symbols, denoted by $PC(\mathbb{T})$ play an important role; see Ref. [53] for more details. Consider a continuous symbol $\lambda : \mathbb{T} \to \mathbb{C}$ and a point $x \notin \mathrm{range}(\lambda)$. There exists a (unique up to some constant offset of the form $2\pi k$ with $k \in \mathbb{Z}$) continuous argument function

$$\arg(\lambda - a) : [-\pi, \pi] \to \mathbb{R}; \phi \mapsto \arg\left[\lambda(\mathrm{e}^{\mathrm{i}\phi}) - a\right]. \tag{70}$$

Independent of the choice of offset, the winding number

$$\mathrm{wind}(\lambda, a) := \frac{1}{2\pi} \arg(\lambda - a)(\pi) - \arg(\lambda - a)(-\pi) \tag{71}$$

is a well-defined integer. Before formulating Szegö's limit theorem, we state an important lemma about the spectrum of Töplitz operators (explaining where the spectrum of the truncated matrices T_n eventually concentrates).

Lemma 5 (Spectrum of Töplitz operators and truncated Töplitz matrices [53]). *Suppose $\lambda \in PC(\mathbb{T})$ and let $T(\lambda)$ be the infinite Töplitz matrix associated to the symbol λ. Assume $U \subseteq \mathbb{C}$ is an open set and assume that the spectrum $\sigma(T(\lambda))$ is a subset of U. Then there exists an index $n_0 \in \mathbb{N}$ such that $n \geq n_0$ implies $\sigma(T_n(\lambda)) \subseteq U$. If λ is continuous the spectrum of $T(\lambda)$ follows entirely from geometric properties of the symbol,*

$$\sigma(T(\lambda)) = \mathrm{range}(\lambda) \cup \{ x \in \mathbb{C} \,|\, \mathrm{wind}(\lambda, x) \neq 0 \}. \tag{72}$$

Szegö's Theorem holds for symbols in the Krein algebra [53]:

Theorem 2 (A second order Szegö theorem [51, 53]). *Let* $\mu \in W \cap B_2^{\frac{1}{2}}$ *be a symbol and let* $T_n \in \mathbb{C}^{n\times n}$ *be the family of associated Töplitz matrices. Let* $\Omega \subseteq \mathbb{C}$ *be an open subset that contains the spectrum of* $T(\mu)$*. For an analytic function* $h : \Omega \to \mathbb{C}$ *the following trace formula holds,*

$$\operatorname{tr}\left(h(T_n)\right) = nG_h(\mu) + E_h(\mu) + o(1) \tag{73}$$

with

$$G_h(\mu) = \frac{1}{2\pi}\int_0^{2\pi} h(\mu(\mathrm{e}^{\mathrm{i}\theta}))d\theta, \tag{74}$$

$$E_h(\mu) = \frac{1}{2\pi\mathrm{i}}\int_{\partial\Omega} h(\lambda)\frac{d}{d\lambda}\log E(\mu-\lambda)d\lambda, \tag{75}$$

$$E(\mu) = \exp\sum_{k=1}^{\infty} k\left(\log\mu\right)_k\left(\log\mu\right)_{-k}, \tag{76}$$

where

$$\left(\log\mu\right)_k := \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{-\mathrm{i}k\theta}\log\mu(\mathrm{e}^{\mathrm{i}\theta})d\theta \tag{77}$$

is the Fourier transform of $\log(\mu)$.

Theorem 3 (Alternative expression for the second order term [52]). *Let* $\mu \in W \cap B_2^{\frac{1}{2}}$ *be absolutely continuous and let* $T_n \in \mathbb{C}^{n\times n}$ *be the family of associated Töplitz matrices. Let* $\Omega \subseteq \mathbb{C}$ *be an open subset that contains the spectrum of* $T(\mu)$ *and let* $h : \Omega \to \mathbb{C}$ *be analytic on* Ω*. Then the second order term* $E_h(\mu)$ *from Theorem 2 can be written as*

$$\begin{aligned} E_h(\mu) = \frac{1}{4\pi^2}\sum_{k=1}^{\infty}\int_{-\pi}^{\pi}d\phi\int_{-\pi}^{\pi}d\theta\,&\frac{h\left(\mu(\mathrm{e}^{\mathrm{i}\theta})\right)-h\left(\mu(\mathrm{e}^{\mathrm{i}\phi})\right)}{\mu(\mathrm{e}^{\mathrm{i}\theta})-\mu(\mathrm{e}^{\mathrm{i}\phi})} \\ &\times\sin\left(k(\theta-\phi)\right)\left(\mu'(\phi)-\mu'(\theta)\right). \end{aligned}$$

Again, the derivative is to be read as in Eq. (37).

Proof of Lemma 1. We are now in the position to prove Lemma 1. We can now collect the results from the previous sections. By the results from Subsection 4.2, specifically Lemma 1, we know that for any subset of sites whose cardinality is much larger than β, we can work with infinite truncated Töplitz matrices and their symbols. The asymptotic expression for the entropy of the full system can be obtained directly from the continuum approximation. Remember that $|A| = \lceil qN\rceil$ and subsystem B is of size $|B| = N - |A|$, where $q \in (0,1)$. Theorem 2 states that the block entropies are asymptotically equal to

$$S_\alpha(\rho_A) = \operatorname{tr}\left(s_\alpha(X|_A)\right) = qNG_{s_\alpha}(\lambda) + E_{s_\alpha}(\lambda) + o(1) \tag{78}$$

and

$$S_\alpha(\rho_B) = \operatorname{tr}\left(s_\alpha(X|_B)\right) = (1-q)NG_{s_\alpha}(\lambda) + E_{s_\alpha}(\lambda) + o(1). \tag{79}$$

We now turn to the computation of the entropy $S_\alpha(\rho)$ of the entire system. This is subtle, and one cannot employ the same formula for the larger system of $A\cup B$: Lemma

1 would no longer be valid, and the boundary conditions would not be respected. But we can still find an asymptotically exact expression. The spectrum of X is given by

$$\left\{(f\circ\varepsilon)(\mathrm{e}^{2\pi\mathrm{i}k/N}) : k=1,\dots,N\right\}. \tag{80}$$

Hence,

$$S(\rho)=\sum_{k\in\mathbb{Z}_N}(s_\alpha\circ f\circ\varepsilon)(\mathrm{e}^{2\pi\mathrm{i}k/N}). \tag{81}$$

Using Lemma 2 again, we find that this expression can be replaced by

$$S(\rho)=NG_s(\lambda)+o(1). \tag{82}$$

Combining the terms, the mutual information is asymptotically equal to

$$I_\alpha(A:B)=2E_{s_\alpha}(\lambda)+o(1). \tag{83}$$

Since the symbol $\mu:=f\circ\varepsilon$ is analytic (and therefore absolutely continuous) Theorem 3 can be applied resulting in the desired expression

$$\begin{aligned}I_\alpha(A:B)=\frac{1}{2\pi^2}\sum_{k=1}^{\infty}\int_{2\pi}^{0}d\phi\int_{2\pi}^{0}d\theta\,\frac{s_\alpha\left(\lambda(\mathrm{e}^{\mathrm{i}\theta})\right)-s_\alpha\left(\lambda(\mathrm{e}^{\mathrm{i}\phi})\right)}{\lambda(\mathrm{e}^{\mathrm{i}\theta})-\lambda(\mathrm{e}^{\mathrm{i}\phi})}\\ \times\sin\left(k(\theta-\phi)\right)\left(\lambda'(\mathrm{e}^{\mathrm{i}\phi})-\lambda'(\mathrm{e}^{\mathrm{i}\theta})\right)+o(1).\end{aligned}$$

which completes the proof. □

4.4. Simplifying Widom's second order expression. We have almost proven the main theorem, but we still need to eliminate the infinite sum in k in Eq. (38). The sum in k is rather awkward; since the integrand is more and more oscillatory for larger and larger k, it is a priori far from clear where one may truncate the sum in order to arrive at a reliable result. In this way, the expression cannot be easily computed, not even numerically, and practically only for low temperatures. We will hence go a technical step further and will prove the validity of Theorem 1, the main result for one-dimensional systems. A first step in this direction is the following observation.

Lemma 6 (Function kernel). *For any $n\in\mathbb{N}$ and any $\phi,\theta\in[0,2\pi)$,*

$$\sum_{1\le k\le n}\sin(k\phi)=\frac{1}{2}\frac{\cos(\phi/2)-\cos((n+1/2)\phi)}{\sin(\phi/2)}=:K_n(\phi). \tag{84}$$

Proof. We first note that the sum over sine functions encountered in Eq. (84) can be brought into a closed form reminiscent of the Dirichlet kernel. Indeed, if we truncate the sum at n, then it can be expressed in closed form as

$$\begin{aligned}\sum_{1\le k\le n}\sin(k\phi)&=\frac{1}{2\mathrm{i}}\sum_{1\le k\le n}(\mathrm{e}^{\mathrm{i}k\phi}-e^{-\mathrm{i}k\phi}) \\ &=\frac{1}{2\mathrm{i}}\sum_{1\le k\le n}\left((\mathrm{e}^{\mathrm{i}\phi})^k-(\mathrm{e}^{-\mathrm{i}\phi})^k\right)\\ &=\frac{1}{2\mathrm{i}}\left(\frac{1-e^{(n+1)\mathrm{i}\phi}}{1-e^{\mathrm{i}\phi}}-\frac{1-e^{-(n+1)\mathrm{i}\phi}}{1-e^{-\mathrm{i}\phi}}\right)\\ &=\frac{1}{2}\frac{\cos\left(\phi/2\right)-\cos\left((n+1/2)\phi\right)}{\sin\left(\phi/2\right)},\end{aligned} \tag{85}$$

where the last line follows from elementary trigonometric identities. □

That is to say, the mutual information can be re-expressed in terms of the kernel K_n as

$$\begin{aligned} I_\alpha(A:B) = \frac{1}{2\pi^2} \lim_{n\to\infty} \int_{-\pi}^{\pi} d\phi \int_{-\pi}^{\pi} d\theta \frac{s_\alpha\left(\lambda(\mathrm{e}^{\mathrm{i}\theta})\right) - s_\alpha\left(\lambda(\mathrm{e}^{\mathrm{i}\phi})\right)}{\lambda(\mathrm{e}^{\mathrm{i}\theta}) - \lambda(\mathrm{e}^{\mathrm{i}\phi})} \\ \times \left(\lambda'(\mathrm{e}^{\mathrm{i}\phi}) - \lambda'(\mathrm{e}^{\mathrm{i}\theta})\right) K_n\left((\theta-\phi)\right) + o(1). \end{aligned} \tag{86}$$

We can further simplify the expression by invoking results from the theory of highly oscillatory integrals. Recall the subsequent fundamental lemma.

Lemma 7 (Riemann-Lebesgue). *Let $f \in L_1([a,b],\mathbb{C})$, let $g \in L_\infty(\mathbb{R},\mathbb{C})$ be periodic (with period T) and assume $\int_0^T g(x)dx = 0$ (the probably most important special instances of such functions g are the trigonometric functions* sin *and* cos*) then*

$$\lim_{n\to\infty} \int_a^b f(t)g(nt)dt = 0. \tag{87}$$

Proof. If $f \in C_C^\infty([a,b],\mathbb{C})$ (hence is a compactly supported smooth function from $[a,b]$ to $\mathbb{C}$), then partial integration gives

$$\int_a^b f(t)g(nt)dt = -\frac{1}{n}\int_a^b f'(t)\int_a^{nt} g(s)dsdt. \tag{88}$$

Note that $f'(t)$ is bounded by assumption and that $|\int_0^{nt} g(s)ds| \leq T\,\|g\|_\infty$ for every $t \in \mathbb{R}$. Hence,

$$\lim_{n\to\infty} \int_a^b f(t)g(nt)dt = 0. \tag{89}$$

For general $f \in L_1([a,b],\mathbb{C})$, note that the smooth, compactly supported functions are dense in $L_1([a,b],\mathbb{C})$. Hence, for an arbitrary $\varepsilon > 0$ there exists $f_2 \in {C_C}^\infty([a,b],\mathbb{C})$ with

$$\|f_2 - f\|_1 \leq \frac{\varepsilon}{\|g\|_\infty (b-a)}. \tag{90}$$

Therefore,

$$\lim_{n\to\infty}\left|\int_a^b f(t)g(nt)dt\right| \leq \lim_{n\to\infty}\left(\left|\int_a^b (f(t)-f_2(t))g(nt)dt\right| + \left|\int_a^b f_2(t)g(nt)dt\right|\right) \leq \varepsilon \tag{91}$$

by validity of the statement for compactly supported, smooth functions. Since $\varepsilon > 0$ was arbitrary, the result also holds true for general $f \in L_1([a,b],\mathbb{C})$. □

This well-known lemma simplifies the understanding of the limiting behaviour of these kernels K_n action on sufficiently regular test functions.

Theorem 4 (Distributional convergence of the kernels K_n). *Let $h \in L_1(\mathbb{T},\mathbb{C})$ be locally Lipschitz continuous at $\mathrm{e}^{\mathrm{i}\theta} \in \mathbb{T}$ then*

$$\lim_{n\to\infty} \int_{-\pi}^{\pi} h(\mathrm{e}^{\mathrm{i}\phi})K_n(\phi-\theta)d\phi = \frac{1}{2}\int_{-\pi}^{\pi} \frac{h(\mathrm{e}^{\mathrm{i}\phi}) - h(\mathrm{e}^{\mathrm{i}\theta})}{\tan\left((\phi-\theta)/2\right)}d\phi. \tag{92}$$

Proof. Without any loss of generality let $\theta = 0$ (otherwise take $\phi' := \phi - \theta$). Assume $h(1) = 0$ first. By Lipschitz continuity of h, there exists some $\varepsilon > 0$ and some constant $L > 0$ such that $\left|h(\mathrm{e}^{\mathrm{i}\phi})\right| < L\,|\phi|$, whenever $|\phi| < \varepsilon$. By continuity, there exists some constant $M > 0$ such that

$$\left|\frac{\phi}{\tan(\phi/2)}\right| < M \tag{93}$$

for $\phi \in [\,-\pi, \pi]$. Therefore

$$\left|\frac{h\left(\mathrm{e}^{\mathrm{i}\phi}\right)}{\tan\left(\phi/2\right)}\right| \le \chi_{(-\varepsilon,\varepsilon)}(\phi)M \cdot L + \chi_{[-\pi,\pi]\setminus(-\varepsilon,\varepsilon)}(\phi)\frac{\left|h(\mathrm{e}^{\mathrm{i}\phi})\right|}{\tan(\varepsilon/2)}, \tag{94}$$

where χ_A is the characteristic function of the (measurable) set A. Define $\tilde{h}(\phi) := h\left(\mathrm{e}^{\mathrm{i}\phi}\right)/\tan\left(\phi/2\right)$. By the previous estimate $\tilde{h} \in L_1([\,-\pi,\pi],\mathbb{C})$ and the Riemann-Lebesgue Lemma can be applied. Applying the Riemann-Lebesgue Lemma twice and using elementary angle-sum identities for trigonometric functions yields

$$\begin{aligned}\lim_{n\to\infty}\int_{-\pi}^{\pi} h(\mathrm{e}^{\mathrm{i}\phi})\frac{1}{2}\frac{\cos(\phi/2)-\cos\left((n+1/2)\phi\right)}{\sin(\phi/2)}d\phi &= \lim_{n\to\infty}\frac{1}{2}\int_{-\pi}^{\pi} h(\mathrm{e}^{\mathrm{i}\phi})\frac{1-\cos(n\phi)}{\tan(\phi/2)}d\phi\\ &= \lim_{n\to\infty}\frac{1}{2}\int_{-\pi}^{\pi}\tilde{h}(\mathrm{e}^{\mathrm{i}\phi})\left(1-\cos(n\phi)\right)d\phi\\ &= \frac{1}{2}\int_{-\pi}^{\pi} h(\mathrm{e}^{\mathrm{i}\phi})\frac{1}{\tan(\phi/2)}d\phi.\end{aligned} \tag{95}$$

If $f(1) \neq 0$ write $h(\mathrm{e}^{\mathrm{i}\phi}) = (h(\mathrm{e}^{\mathrm{i}\phi}) - h(1)) + h(1)$, apply the former result to the first summand and note that

$$\int_{-\pi}^{\pi}\frac{\cos(\phi/2)-\cos\left((n+1/2)\phi\right)}{\sin(\phi/2)}d\phi = 0, \tag{96}$$

for every $n \in \mathbb{N}$ by anti-symmetry of the integrand. $\square$

We need an extension to double integrals, a proof of which follows the same line of reasoning.

Theorem 5 (Distributional convergence of the kernels K_n for double integrals). *Let $h \in L_1(\mathbb{T}^2,\mathbb{C})$ be Lipschitz continuous in a neighborhood of the diagonal*

$$D_{\mathbb{T}^2} := \left\{(x,y)\in\mathbb{T}^2\,|x=y\right\} \tag{97}$$

then

$$\lim_{n\to\infty}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} h(\mathrm{e}^{\mathrm{i}\phi},\mathrm{e}^{\mathrm{i}\theta})K_n(\phi-\theta)d\phi d\theta = \frac{1}{2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{h(\mathrm{e}^{\mathrm{i}\phi},\mathrm{e}^{\mathrm{i}\theta})-h(\mathrm{e}^{\mathrm{i}\theta},\mathrm{e}^{\mathrm{i}\theta})}{\tan\left(\frac{\phi-\theta}{2}\right)}d\phi d\theta. \tag{98}$$

As a consequence, Eq. (86) can be rewritten in the following way:

$$I_\alpha(A:B) = \frac{1}{4\pi^2}\int_{-\pi}^{\pi} d\phi \int_{-\pi}^{\pi} d\theta \frac{s_\alpha\left(\lambda(\mathrm{e}^{\mathrm{i}\theta})\right) - s_\alpha\left(\lambda(\mathrm{e}^{\mathrm{i}\phi})\right)}{\lambda(\mathrm{e}^{\mathrm{i}\theta}) - \lambda(\mathrm{e}^{\mathrm{i}\phi})} \frac{(\lambda'(\phi) - \lambda'(\theta))}{\tan((\phi-\theta)/2)} + o(1). \tag{99}$$

Let us conclude this subsection by commenting on the second order term in the trace formula of Theorem 3. Recently, another related approach aiming at a simplification of Widom's formula has been discussed in the literature. The main result of a recent masters' thesis [56] is a derivation of a second order trace formula from asymptotic inverses and appropriate factorisations of the symbol. The presented final expression of the second order term does not contain k-sum as well and finally only involves the calculation of an appropriate double integral – a result similar to ours. However, the given double integral always involves complex valued integration whereas our formula contains only real valued integrands right from the beginning (whenever the symbol is real-valued and the analytic function restricted to the reals is also real-valued as usually satisfied in problems of practical relevance).

Indeed, the idea to approach the trace formula starting with the inverse function rather then the usual logarithm (the term $E(\mu)$ from Szegö's theorem is just the second order term of the logarithm) has many didactical and computational advantages in our opinion. First of all, this computationally inappropriate and practically incomputable $k-$sum in $E_h(\mu)$ is missing right from the beginning – note that for larger and larger k, the integrand becomes more and more oscillatory in a fashion that is hard to grasp. Furthermore, there exist well-known asymptotic expansions for asymptotic inverses even for higher order terms (which are very useful for approximate solutions of systems of linear equation with coefficient matrix being a Töplitz matrix for example). Last but not least the authors of Ref. [56] were able to derive second order formulas for block Töplitz matrices (which require – unlike the final result in the one-dimensional setting – an explicit factorisation of $\lambda\mathbb{1} - \mu$ where μ is the matrix-valued symbol and λ is an arbitrary complex number on the integration contour).

5. Temperature dependence

5.1. General remarks. Our main result, Theorem 4.1, gives an asymptotically exact expression for the mutual information of two neighbouring blocks of fermions in one dimension. It has been shown that for a given inverse temperature $\beta > 0$,

$$I_\alpha(A:B) = I_{\alpha,\infty}(A:B) + o(1) \tag{100}$$

in the system size N. The result given constitutes an easily computable expression that paves the way for studying a number of physically meaningful regimes. At this point, we would like to pause for a moment, however, and would like to come back to one of the questions posed in the introduction, namely of the possible asymptotic behaviour of $I_{\alpha,\infty}(A:B)$ for large and small inverse temperatures. As we have seen above, the general bound of Ref. [42] following from the extremality of the free energy suggests that the mutual information should scale like β for large temperatures,

$$I_{\alpha,\infty}(A:B) = O(\beta). \tag{101}$$

One might wonder whether this bound actually gives the proper asymptotic scaling on the temperature. Conformal field theory actually suggests a behaviour which is logarithmic rather than linearly in the inverse temperature [2, 27]. In this section, we corroborate the prediction from conformal field theory by showing that the low temperature

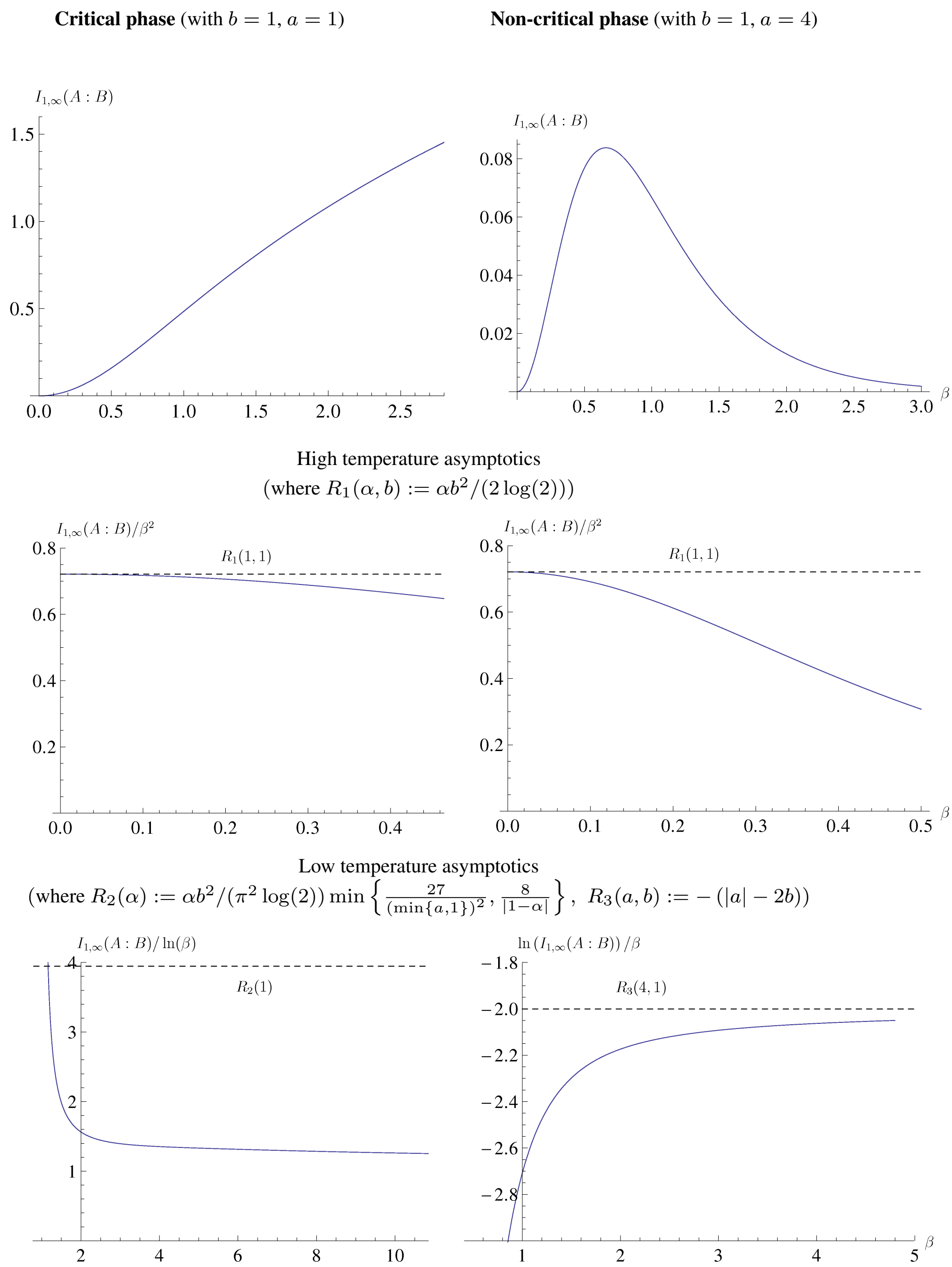

Fig. 2. Temperature dependence of the von-Neumann mutual information for various parameters of the fermionic instance of the XX model.

asymptotics are given by

$$I_{\alpha,\infty}(A:B) = O(\log(\beta)). \tag{102}$$

This has a quite remarkable consequence: In order to see features of the criticality of the ground state, one has to go to extremely low temperatures. This dependence is also convincingly depicted in Fig. 2, where a logarithmic scale has been chosen – otherwise, signatures of ground state features could hardly be detected. Only at extraordinarily low temperatures, the familiar logarithmic divergence in the system size of the sub-block chosen becomes visible for a reasonably sized subsystem.

5.2. Analysis of the XX model. Needless to say, the low temperature asymptotics depends on the choice of the model parameters a and b. Specifically, the scaling of the mutual information reflects signatures of the zero temperature quantum phase transition of this model taking place at $|a| = 2b$. Whenever $|a| < 2b$ the model is critical in its ground state, i.e., there is no energy gap. It is known that the entanglement entropy then exhibits a logarithmic divergence – signatures of that are also seen in the mutual information at small but non-zero temperature. If the model is gapped, i.e., whenever $|a| > 2b$, the ground state is the vacuum or the fully occupied state, depending on the sign of a. As expected, the mutual information converges exponentially quickly to zero in the non-critical phase at a rate proportional to the energy gap. The main insights for this model are summarised in the following theorem:

Theorem 6 (Temperature dependence). *The ($\alpha-$) mutual information of the thermal state of the fermionic XX model with parameters $a \in \mathbb{R}$ and $b > 0$ satisfies*

$$\lim_{\beta\to 0} \frac{I_{\alpha,\infty}(A:B)}{\beta^2} = \frac{\alpha b^2}{2\log(2)}. \tag{103}$$

Whenever $|a| < 2b$, then

$$\begin{aligned}&\limsup_{\beta\to\infty} \frac{I_{\alpha,\infty}(A:B)}{\log\beta} \\ &\leq \frac{2\alpha}{\pi^2\log(2)\left(\min\{1,\alpha\}\right)^2} \min\left\{\frac{27}{2\left(\min\{1,\alpha\}\right)}, \frac{4}{|1-\alpha|}\right\}.\end{aligned} \tag{104}$$

Whenever $|a| > 2b$, then for any $\kappa < (|a| - 2b) \cdot \min\{\alpha, 1\}$

$$\lim_{\beta\to\infty} \exp(\kappa\beta) I_{\alpha,\infty}(A:B) = 0. \tag{105}$$

The proof of this statement is rather involved and requires a number of techniques developed in lemmas: Hence, for better readability of the main text, it will be presented in the appendix in Subsection 8.4.

6. Free fermonic models on the torus

The results established above readily apply to the situation of a bi-sected, higher-dimensional fermionic lattice system on the torus. A quite similar strategy has already been exploited, e.g., in Ref. [25]. Using appropriate discrete Fourier transforms, one can disentangle the constituents from each other with respect to all but one dimensions. The exception is the dimension in which the two regions labeled A and B are singled out, see Fig. 3. In this way, one arrives at a collection of suitably modulated and altered one-dimensional problems, to which the above statements apply. In this section, we highlight the results obtained in this manner. An important application of this is the computation of the mutual information in *higher-dimensional tight binding models*.

6.1. Geometry of the problem. Let us for simplicity consider in D dimensions the geometry of slabs $L = (\mathbb{Z}_M)^{D-1} \times \mathbb{Z}_N$, for suitable N and M. So along one dimension, we have as before N sites, whereas the system size with respect to the other dimensions is M, see Fig. 3. The index set of all sites can be taken to be

$$I = I' \times J, \tag{106}$$
$$I' = \{0, \ldots, M-1\}^{\times D-1}, \tag{107}$$
$$J = \{0, \ldots, N-1\}. \tag{108}$$

Vectors of indices $i \in I \subset \mathbb{Z}^D$ will be regarded as modulo N and M, respectively. Let $w : \mathbb{Z}^D \to L$ be defined as

$$w(i) = w(i_1, \ldots, i_D) = (i_1 \mathrm{mod} M, \ldots, i_{D-1} \mathrm{mod} M, i_D \mathrm{mod} N). \tag{109}$$

This function simply projects arbitrary indices from $\mathbb{Z}^D$ onto the lattice L. We again allow for arbitrary finite-ranged interactions (the generalization to exponentially decaying interactions is straightforward but omitted). That is to say, for $i, j \in I$, the Hamiltonian tensor takes the form

$$V^i_j = d_{w(i-j)}. \tag{110}$$

Then the Hamiltonian can be written in the following way

$$H := \sum_{i,j \in I} V^i_j f^\dagger_i f_j = \sum_{a,b \in I'; c,d \in J} V^{(a,c)}_{(b,d)} f^\dagger_{(a,c)} f_{(b,d)}. \tag{111}$$

We have singled our the special spatial dimension for which we consider the bi-partite cut. We take the parts A and B to be

$$A = I' \times \{0, 1, \ldots, \lceil qN \rceil - 1\}, \tag{112}$$
$$B = I' \times \{\lceil qN \rceil, \lceil qN \rceil + 1, \ldots, N-1\}, \tag{113}$$

with q as before. We will also see that the previously found results still apply.

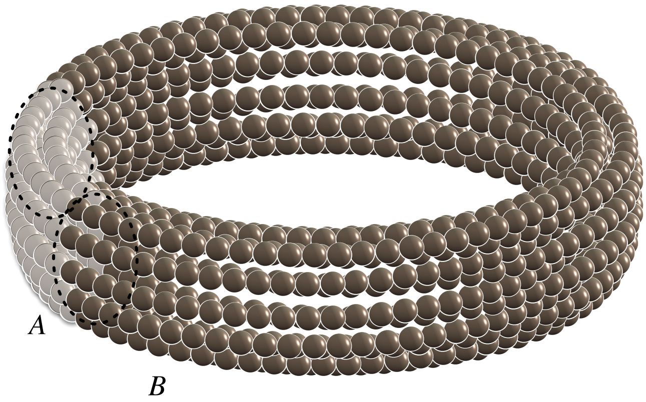

Fig. 3. The geometry of the free fermionic model on the torus. Along a singled out dimension, the system consists of N sites, while the other dimensions with the topology of a torus embody M sites. The distinguished region is again referred to as A, its complement is B.

6.2. Scaling of the mutual information on the torus. We can now consider Fourier transforms with respect to the index set I', while leaving the index set J invariant. For the discrete Fourier transform, we choose

$$U_{k,l} := \frac{1}{\sqrt{M^{D-1}}} \exp\left(\frac{2\pi \mathrm{i}}{M^{D-1}} k \cdot l\right) \text{ for } k, l \in I'. \tag{114}$$

It can then be shown that

$$\begin{aligned} V'^{(k,k_0)}_{(l,l_0)} &:= \left((U \otimes \mathbb{1}) \left(V^i_j\right)_{i,j} \left(U^\dagger \otimes \mathbb{1}\right)\right)_{(k,k_0),(l,l_0)} \\ &= \underbrace{\left(\sum_{t \in I'} \exp\left(\frac{2\pi \mathrm{i}}{N'} t \cdot l\right) d_{(t,k_0-l_0)}\right)}_{:=\tilde{d}^{(l)}_{k_0,l_0}} \delta_{k,l}. \end{aligned} \tag{115}$$

That is to say, the reduced entropies of A and B as well as the global entropy can be computed as if one had uncoupled one-dimensional systems, only that the coupling is modulated in a way described by the new couplings in Eq. (115). Denote for $k \in I'$ the resulting expression of the symbol computed from $\tilde{d}^{(k)}$

$$\lambda_k = f \circ \varepsilon_k, \tag{116}$$

where ε_k is the expression as defined in Eq. (20), with d replaced by $\tilde{d}^{(k)}$ for each k. In this way, we also arrive at the asymptotically exact expression for the mutual information in the limit of large N, recovering the logarithmic divergence of the mutual information.

Theorem 7 (Mutual information on the torus). *For any inverse temperature $\beta > 0$, any $M \in \mathbb{N}$, and for any $\alpha \in [0, \infty)$, the mutual information is given by the, in N*

asymptotically exact, expression

$$I_\alpha(A:B) = \frac{1}{4\pi^2} \sum_{k\in I'} \int_{-\pi}^{\pi} d\phi \int_{-\pi}^{\pi} d\theta \\ \times \frac{s_\alpha(\lambda_k(\mathrm{e}^{\mathrm{i}\theta})) - s_\alpha(\lambda_k(\mathrm{e}^{\mathrm{i}\phi}))}{\lambda_k(\mathrm{e}^{\mathrm{i}\theta}) - \lambda_k(\mathrm{e}^{\mathrm{i}\phi})} \frac{\lambda_k'(\phi) - \lambda_k'(\theta)}{\tan((\theta-\phi)/2)} + o(1). \tag{117}$$

In particular, in this way, we find for tight binding models on the torus in any dimension D that

$$I(A:B) = O(M^{D-1}\log(\beta)) \tag{118}$$

for large inverse temperatures β: The logarithmic divergence in the inverse temperature remains, while an additional term relating to an area law in D dimensions emerges.

7. Outlook

7.1. Conformal field theory and entanglement spectra. In this section, we compare our results with predictions from *conformal field theory*. Indeed, our findings can be seen as a confirmation of the predictions resulting from the conformal transformation relating finite systems at zero temperature to infinite systems at finite temperature. In our result, we provide system specific qualifiers of the asymptotic limits, and our main theorem constitutes a fully rigorous result applicable to a large class of models. Also, higher-dimensional systems on tori can be captured with the methods presented here. Still, it is interesting to see that the behaviour of the mutual information, scaling asymptotically as the logarithm in the inverse temperature, can also immediately be suggested from the analysis of conformal field theories in $1+1$ dimensions. This is an observation similar to the one made for ground state properties of the XX model in the ground state [10, 26]: Here, the rigorous expression given relates to and confirms the formula [2, 6]

$$S_A = \frac{c}{3}\log\frac{l}{a} + c_1, \tag{119}$$

in a connection already conjectured in Ref. [8]. Here, $c_1 > 0$ is a constant and a is the lattice spacing, while c is the conformal charge. The results on entanglement entropies in the XX models were proven using Fisher-Hartwig type methods for Töplitz determinants [10, 26].

The main idea in the conformal analysis is that there exists a connection between correlation properties of finite systems at zero temperature and infinite systems at finite temperature. Therefore, assume that at zero temperature, the entanglement entropy scales as

$$S_A = f(l) \tag{120}$$

for some function $f:\mathbb{R}^+ \to \mathbb{R}^+$. Then, at large inverse temperatures $\beta > 0$, we consider the conformal mapping $z \mapsto \mathrm{e}^{2\pi z/(v\beta)}$ for $v > 0$, to arrive at the expression [27]

$$S_A = f\left(\frac{v\beta}{\pi}\sinh\left(\frac{\pi l}{v}\right)\right). \tag{121}$$

Combined with Eq. (120), one hence gets for $\beta > 0$ [2, 27]

$$S_A = \frac{c}{6}\log\left(\frac{\beta}{\pi a}\sinh\left(\frac{2\pi l}{\beta}\right)\right) + c_3, \tag{122}$$

for $c > 3 > 0$. The above statement becomes meaningful in the limit when $l \gg \beta$. Asymptotically, S_A is well approximated by $\pi c l/(3\beta) + c_3$ [2], but for our purposes, we also need a first order correction, namely

$$S_A \approx \frac{c}{6}\left(\log\left(\frac{\beta}{\pi a}\right) - \log(2) + \frac{2\pi l}{\beta}\right) + c_3. \tag{123}$$

In this way, one recovers the expression for the mutual information

$$I(A:B) \approx \frac{c}{3}\log\left(\frac{\beta}{\pi a}\right), \tag{124}$$

again exhibiting a logarithmic dependence in β, as $\beta \to \infty$. The analysis of the finite temperature case axing arguments from conformal field theory has recently been carried out in Refs. [58, 59]. As mentioned earlier, the criticality of the ground state is not felt by the mutual information, unless one is at extremely low temperatures. In turn, the logarithmic scaling in the size of a subregion is turned into a logarithmic dependence on the inverse temperature.

It is important to note that because the formalism developed here allows for the computation of all Renyi entropies, the tools developed in this paper also allow for the study spectra of reductions; i.e. *entanglement spectra* [36–41], compare also Refs. [1, 2]. Such entanglement spectra have turned out to provide a powerful tool when characterizing *topological order*, relating bulk to boundary theories, and discussing the possibility of approximating states with suitable *tensor network states* such as *matrix product states and operators* and higher-dimensional analogues.

7.2. Remarks on open free fermionic many-body systems. Let us finally briefly mention that the formalism developed here in principle also allows for the study of *open quantum systems*, undergoing dissipation and quantum noise. An extensive discussion of this topic is beyond the scope of the present article. In the mindset developed here, one can consider *Liouvillians* capturing fermionic open quantum systems of the form

$$\mathcal{L}(\rho) = \mathrm{i}[H,\rho] + \sum_{j\in\mathbb{Z}_N}\left(L_j\rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j,\rho\}\right) \tag{125}$$

with, as before,

$$H = \sum_{i,j\in\mathbb{Z}_N} f_j^\dagger V_{j,k} f_k, \tag{126}$$

and the L_j are operators linear in the fermionic operators, supported on finitely many sites only, which are all the same, except that they are all translates of each other. The Lindblad operators L_j hence act locally in the same way as the Hamiltonian terms act locally. The equations of motions then become

$$\frac{d}{dt}\rho(t) = \mathcal{L}(\rho). \tag{127}$$

A state ρ is called a steady state if $\mathcal{L}(\rho) = 0$. For fully translationally invariant systems, one can again define a symbol [44, 45], and the methods developed here are applicable. Details of such an approach will be pursued elsewhere. Such an idea seems particularly timely in the light of the observation that open system dynamics should not only be

viewed as a source of quantum noise added to the system. But that open system dynamics and dissipation can also be beneficial: Indeed, dissipative dynamics allows for dissipative instances of quantum information processing [46–48], exhibiting an interesting way of protection. Also, steady states can readily exhibit a number of exciting properties: they can be *entangled*, show phenomena of *noise-driven criticality*, or even exhibit *topological order* [44–46]. The latter is specifically true for free fermionic models, an arena for which the machinery developed here should be fruitful.

7.3. Summary. In this work, we have introduced a formalism allowing us to prove the validity of rigorous expressions for the Renyi mutual information of Gibbs states of translationally invariant quasi-free fermionic models. The expressions obtained are asymptotically exact; the bounds given are also exponentially tighter than those derived from the extremality of the Gibbs state with respect to the free energy. Special emphasis has been put onto the technical development of novel methods of dealing with Töplitz matrices, in particular a new and useful instance of a second order expression for smooth symbols. These tools, as well as the approximation results introduced here, are expected to be widely applicable and highly useful in various contexts. It is the hope that this work inspires further entanglement-related studies of mixed fermionic quantum states, arising in the context of describing both closed and open quantum many-body systems.

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8. Appendix

8.1. Simple and useful upper and lower bounds to the mutual information. In this subsection, we will derive upper and lower bounds to the quantum mutual information, evaluated for Gaussian fermionic states. These bounds are generally useful when bounding mutual information expressions. Moreover, they are additive, so share this important feature with the actual mutual information. We expect these bounds to be useful also in other contexts, different from the study pursued here. What is more, it should be clear that one can immediately also formulate a bosonic variant of the bounds presented here, using the same strategy of proof. We consider covariance matrices $\gamma \in \mathbb{R}^{2n\times 2n}$ of the form

$$\gamma = \begin{pmatrix} 0 & X \\ -X & 0 \end{pmatrix}, \tag{128}$$

with $X = X^T$. We write

$$X = \begin{pmatrix} X_A & X_{AB} \\ X_{BA} & X_B \end{pmatrix} \tag{129}$$

and denote with P the pinching [55]

$$P = \begin{pmatrix} X_A & 0 \\ 0 & X_B \end{pmatrix} = X_A \oplus X_B \tag{130}$$

of X. This is the covariance matrix of the tensor product of the two reduced states, as a moment of thought reveals. In these terms, the quantum mutual information can hence be written as

$$I(A:B) = \mathrm{tr}(s(P)) - \mathrm{tr}(s(X)), \tag{131}$$

so as a difference of two trace functions. Let us now consider a quadratic function $l : [-1,1] \to [0,1]$ defined as

$$l(x) = (1-x^2)/2. \tag{132}$$

We will see that the corresponding difference of trace functions is a convenient, computable lower bound of the mutual information with reasonable properties. We hence relate the mutual information to *purities* only (or, for that matter, to 2-Renyi mutual informations)[2].

[2] It may be important to state that since these quantities only referring to local and global purities are easier to measure, these bounds are expected to be useful even in an experimental context.

Lemma 8 (Lower bound to the mutual information). *For any $X = X^\dagger$,*

$$\mathrm{tr}(s(P)) - \mathrm{tr}(s(X)) \geq \mathrm{tr}(l(P)) - \mathrm{tr}(l(X)). \tag{133}$$

Moreover, the bound is additive, in that

$$\mathrm{tr}(l(P)) = \mathrm{tr}(l(X_A)) + \mathrm{tr}(l(X_B)). \tag{134}$$

Proof. To start with, the additivity immediately follows from the definition. We have

$$\begin{aligned}\mathrm{tr}(l(P)) &= \frac{1}{2}\mathrm{tr}(\mathbb{1}_{2n} - (X_A \oplus X_B)^2) \\ &= \frac{1}{2}\mathrm{tr}(\mathbb{1}_{2n} - (X_A^2 \oplus X_B^2)) \\ &= \mathrm{tr}(l(X_A)) + \mathrm{tr}(l(X_B)).\end{aligned} \tag{135}$$

This lower bound as such can be shown using a result of the theory of convex trace functions called Peierls' inequality [55]. The function $s - l$ is a concave function (it is not required that it is operator concave). What is more, we can without loss of generality assume that X_A and X_B are both diagonal. If they are not, there exist real orthogonal matrices O_A, O_B such that $(O_A \oplus O_B)P(O_A \oplus O_B)^T$ is diagonal, without altering the value of the mutual information or the bound. Using the concavity of $g := s - l$, we find

$$\sum_j g(X_{j,j}) \geq \mathrm{tr}(g(X)). \tag{136}$$

But since X_A and X_B are diagonal, we have

$$\mathrm{tr}(g(P)) \geq \mathrm{tr}(g(X)) = \mathrm{tr}(s(X)) - \mathrm{tr}(l(X)) \tag{137}$$

which is what we intended to show. $\square$

Note the similarity of this bound for the mutual information with the bound presented in Ref. [14] for the von-Neumann entropy. It is quite remarkable that this bound can even be used for differences of entropies, not only of entropies as such.

We now turn to upper bounds. Let us define the function $u : [-1, 1] \to [0, 1]$ as

$$u(x) = \frac{1}{\log(2)}(1 - x^2)^{1/2}. \tag{138}$$

Again, one can prove that the upper bound derived from this matrix function, $\mathrm{tr}(u(P)) - \mathrm{tr}(u(X))$ shares the above additivity property. Again, one can prove in the same way as above that one encounters an upper bound. Of course, the function $u - s$ is no longer concave, but convex, so $l - s$ is concave. This bound is not a quadratic bound any more. Using again Peierls' inequality, one arrives at the following result.

Lemma 9 (Upper bound to the mutual information). *For any $X = X^\dagger$,*

$$\mathrm{tr}(s(P)) - \mathrm{tr}(s(X)) \leq \mathrm{tr}(u(P)) - \mathrm{tr}(u(X)). \tag{139}$$

The bound is additive,

$$\mathrm{tr}(l(P)) = \mathrm{tr}(u(X_A)) + \mathrm{tr}(u(X_B)). \tag{140}$$

This upper bound on the mutual information is a very useful bound in its own right.

8.2. Derivatives of entropy functions. For convenience, we present the derivatives of the entropy functions used here.

Lemma 10 (Derivatives of the entropy functions). *The derivatives of the entropy functions are given by*

$$s'_\alpha(x) = \frac{\alpha}{(1-\alpha)\log(2)} \frac{(1+x)^{\alpha-1} - (1-x)^{\alpha-1}}{(1+x)^\alpha + (1-x)^\alpha}, \tag{141}$$

$$s''_\alpha(x) = -\frac{\alpha}{\log(2)} \left(\frac{(1+x)^{\alpha-2} + (1-x)^{\alpha-2}}{(1+x)^\alpha + (1-x)^\alpha} \right.$$
$$\left. + \frac{\alpha}{1-\alpha} \left(\frac{(1+x)^{\alpha-1} - (1-x)^{\alpha-1}}{(1+x)^\alpha + (1-x)^\alpha} \right)^2 \right), \tag{142}$$

$$s'(x) = \frac{1}{2} \log_2 \left(\frac{1-x}{1+x} \right), \tag{143}$$

$$s''(x) = -\frac{1}{\log(2)} \left(\frac{1}{1+x} + \frac{1}{1-x} \right). \tag{144}$$

8.3. Second order theorem for convex functions of Töplitz operators. In this subsection, we elaborate on second order theorems for convex functions of self-adjoint Töplitz operators. It builds upon the analysis of the main text, but is not directly required in any of the above proofs. For the main statement of this subsection, we will need Peierls' inequality in the following form.

Lemma 11 (Peierl's inequality). *Let $A = A^\dagger$ be a Hermitian $N \times N$ matrix and let U be a unitary $N \times N$ matrix. Then, for any function f that is convex on some open interval I with $\sigma A \in I$, one finds that*

$$\sum_{1 \le i \le N} f\left(\left(UAU^\dagger\right)_{ii} \right) \le \operatorname{tr} f(A). \tag{145}$$

The following statement holds.

Theorem 8 (Self-adjoint Töplitz operators). *Let $\mu \in W \cap B_2^{\frac{1}{2}}$ be a symbol. Assume further that $\operatorname{range}(\mu) \subseteq \mathbb{R}$ (or equivalently assume that $T(\mu) = T(\mu)^\dagger$). Then the associated family of Töplitz matrices, $T_n \in \mathbb{C}^{n\times n}$ is Hermitian. Let $J \subseteq \mathbb{R}$ be an open interval with $\operatorname{range}(\mu) \subseteq J$ and let $h : J \to \mathbb{R}$ be real- analytic. Then there exists an analytic extension $\tilde{h}$ of h to a small complex neighborhood of $\tilde{J}$ of $\operatorname{range}(\mu)$ with $\tilde{h}\,\big|_{\operatorname{range}(\mu)} = h\,\big|_{\operatorname{range}(\mu)}$ (compare Lemma 2) and the trace formula of Theorem 2 holds true for this extension. Moreover if h is convex, then*

$$E_h(\mu) \le 0 \tag{146}$$

Proof. The only non-obvious statement is

$$E_h(\mu) \le 0 \tag{147}$$

Fix $\varepsilon > 0$ and $n_0 \in \mathbb{N}$ large enough such that

$$\operatorname{tr} h(T_n) = nG_h(\mu) + E_h(\mu) + r_n \tag{148}$$

with $|r_n| < \varepsilon/3$ for every $n \geq n_0$. Since T_n is Hermitian we have $r_n \in \mathbb{R}$. Choose unitary matrices U that diagonalize T_{n_0}. Then

$$2h(T_{n_0}) = \sum_{1 \leq i \leq 2n_0} h\left(\left(U \oplus UT_{2n_0}U^\dagger \oplus U^\dagger\right)_{ii}\right) = 2n_0 G_h(\mu) + 2E_h(\mu) + 2r_{n_0}. \tag{149}$$

Hence, by Peierl's inequality:

$$2nG_h(\mu) + 2E_h(\mu) + 2r_{n_0} \leq \operatorname{tr}\left(h\left(T_{2n_0}\right)\right) = 2n_0 G_h(\mu) + E_h(\mu) + r_{2n_0}. \tag{150}$$

Therefore:

$$E_h(\mu) \leq r_{2n_0} - 2r_{n_0} < \varepsilon. \tag{151}$$

Since $\varepsilon > 0$ was arbitrary this implies

$$E_h(\mu) \leq 0. \tag{152}$$

□

Since obviously $E_{h_1+h_2}(\mu) = E_{h_1}(\mu) + E_{h_2}(\mu)$ and $E_{\lambda h}(\mu) = \lambda E_h(\mu)$ for $\lambda \in \mathbb{C}$ this implies that $E_{h_1}(\mu) \leq E_{h_2}(\mu)$ whenever $h_1 - h_2$ is convex. If both h_1 and h_2 are differentiable twice this holds true if and only if $h_1'' \leq h_2''$.

8.4. Proof of Theorem 6.

Proof. We start with proving the part of the theorem relating to the high temperature dependence, Eq. (103)). For that purpose, we formulate the explicit asymptotic expression for the mutual information of a thermal state of the fermionic instance of the XX model. Define

$$\epsilon_\beta(\phi) := \beta\left(\frac{a}{2} + b\cos(\phi)\right). \tag{153}$$

Then

$$\epsilon'_\beta(\phi) := -\beta b \sin(\phi). \tag{154}$$

The symbol takes the form $\lambda(\mathrm{e}^{\mathrm{i}\phi}) = -\tanh(\epsilon_\beta(\phi))$. In these terms, we can express the mutual information as

$$I_{\alpha,\infty}(A:B) = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\theta d\phi f_\beta(\theta,\phi) t_\beta(\theta,\phi), \tag{155}$$

where we have decomposed the integrand into the functions

$$\begin{aligned} f_\beta(\theta,\phi) &:= \frac{s_\alpha(\tanh(\epsilon_\beta(\theta))) - s_\alpha(\tanh(\epsilon_\beta(\phi)))}{\tanh(\epsilon_\beta(\theta)) - \tanh(\epsilon_\beta(\phi))} \qquad (156)\\ &\times \left(\frac{\epsilon'_\beta(\theta)}{\cosh^2\left(\epsilon_\beta(\theta)\right)} - \frac{\epsilon'_\beta(\phi)}{\cosh^2\left(\epsilon_\beta(\phi)\right)}\right), \\ t_\beta(\theta,\phi) &:= \tan^{-1}\left(\frac{\theta-\phi}{2}\right). \qquad (157) \end{aligned}$$

The high temperature (small β) limit can be calculated simply by expanding the functions in the integrand, to leading non-zero order in β, which yields

$$f_\beta(\theta,\phi) = \frac{\alpha b \beta^2}{2\log(2)} \left(a + b\left(\cos\theta + \cos\phi\right)\right)\left(\sin\theta - \sin\phi\right) + O(\beta^3). \tag{158}$$

Now, noting that

$$\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\theta d\phi \left(a + b\left(\cos\theta + \cos\phi\right)\right)\left(\sin\theta - \sin\phi\right)\tan^{-1}\left((\theta-\phi)/2\right) = 4b\pi^2, \tag{159}$$

we find that

$$\lim_{\beta\to 0}\frac{I_{\alpha,\infty}(A:B)}{\beta^2} = \frac{\alpha b^2}{2\log(2)}. \tag{160}$$

□

The second part of the theorem, relating to the low temperature asymptotics (i.e., the asymptotics for large β), turns out to be significantly more involved. In a first step, we will cast the integral into a more appropriate form. By an elementary argument involving the symmetry of the problem, one finds that

$$I_{\alpha,\infty}(A:B) = \frac{1}{2\pi^2}\left(I_1 + I_2\right), \tag{161}$$

where

$$I_1 = \int_0^\pi\int_0^\pi d\theta d\phi f_\beta(\theta,\phi) t_\beta(\theta,\phi), \tag{162}$$

and

$$I_2 = \int_0^\pi\int_{-\pi}^0 d\theta d\phi f_\beta(\theta,\phi) t_\beta(\theta,\phi), \tag{163}$$

In this expression, we have made use of the same notation as in the above proof of the low temperature behavior. Note that both $\cos$ functions are monotonous functions of there argument in both regions of integration. The substitution

$$x := \cos(\theta), \tag{164}$$

$$y := \cos(\phi). \tag{165}$$

and an appropriate rearrangement of factors then gives

$$I_1 = \beta b \int_{-1}^{1}\int_{-1}^{1} dx dy f_{\beta,11}(x,y)\left(f_{\beta,12}(x,y) + f_{\beta,13}(x,y)\right), \tag{166}$$

where

$$f_{\beta,11}(x,y) := \frac{s_\alpha(\tanh(\tilde\epsilon_\beta(x))) - s_\alpha(\tanh(\tilde\epsilon_\beta(y)))}{x-y}, \tag{167}$$

$$f_{\beta,12}(x,y) := \frac{\operatorname{sech}^2(\tilde\epsilon_\beta(x))\left(1-x^2\right) - \operatorname{sech}^2(\tilde\epsilon_\beta(y))\left(1-y^2\right)}{\tanh(\tilde\epsilon_\beta(x)) - \tanh(\tilde\epsilon_\beta(y))}\frac{1}{(1-x^2)^{1/2}(1-y^2)^{1/2}}, \tag{168}$$

$$f_{\beta,13}(x,y) := \frac{\operatorname{sech}^2(\tilde\epsilon_\beta(x)) - \operatorname{sech}^2(\tilde\epsilon_\beta(y))}{\tanh(\tilde\epsilon_\beta(x)) - \tanh(\tilde\epsilon_\beta(y))}. \tag{169}$$

In this equation, we have defined

$$\tilde{\epsilon}_\beta(x) := \beta(a/2 + bx). \tag{170}$$

An analogous computation for I_2 yields:

$$I_2 = \beta b \int_{-1}^{1}\int_{-1}^{1} dxdy f_{\beta,11}(x,y)\left(f_{\beta,12}(x,y) - f_{\beta,13}(x,y)\right). \tag{171}$$

We need the following elementary but powerful lemma.

Lemma 12 (Bounds on difference quotients). *Let f, g, h, k be differentiable functions on some open interval $I \subseteq \mathbb{R}$. Assume*

- *$s'(z) \geq 0$ for any $s \in \{f, g, h, k\}$ and any $z \in I$,*
- *$\sup\{s'(z)\,|z \in I\} < \infty$ for any $s \in \{f, g, h, k\}$,*
- *$f'(z) \leq h'(z)$ and $k'(z) \leq g'(z)$ for all $z \in I$.*

Then, for any pair of real numbers $x, y \in I$ with $x \neq y$,

$$0 \leq \frac{f(x) - f(y)}{g(x) - g(y)} \leq \frac{h(x) - h(y)}{k(x) - k(y)}. \tag{172}$$

Proof. By the mean value theorem there exists some $z \in I$ with $x < z < y$ such that

$$\frac{(h-f)(x) - (h-f)(y)}{x - y} = h'(z) - f'(z) \geq 0. \tag{173}$$

Hence

$$\frac{h(x) - h(y)}{x - y} \geq \frac{f(x) - f(y)}{x - y} \geq 0, \tag{174}$$

where the last inequality follows from $f' \geq 0$. By the same argument

$$\frac{g(x) - g(y)}{x - y} \geq \frac{k(x) - k(y)}{x - y} \geq 0, \tag{175}$$

multiplying both inequalities and rearranging terms yields the desired lemma. □

Moreover, we will use the following integral.

Lemma 13 (Integral over exponential difference quotient). *For any $a_1 < a_2$ and $b_1 < b_2$,*

$$\begin{aligned} A_{a_1,a_2,b_1,b_2} &:= \int_{a_1}^{a_2}\int_{b_1}^{b_2} dxdy \frac{\exp(-x) - \exp(-y)}{y - x} \\ &= F(b_1, a_1, a_2) + F(a_1, b_1, b_2) - F(b_2, a_1, a_2) - F(a_2, b_1, b_2). \end{aligned} \tag{176}$$

Here

$$F(a, b, c) := \exp(-a)\left[\tilde{F}(b - a) - \tilde{F}(c - a)\right] \tag{177}$$

with

$$\tilde{F}(x) := \mathrm{Ei}[-x] - \log|x| = \lambda_E + \sum_{k\geq 1} \frac{(-1)^k z^k}{kk!} \tag{178}$$

where

$$\mathrm{Ei}(x) := \int_{-\infty}^{x} \frac{\exp(t)}{t} \tag{179}$$

is the exponential integral function and γ_E denotes the Euler Gamma constant.

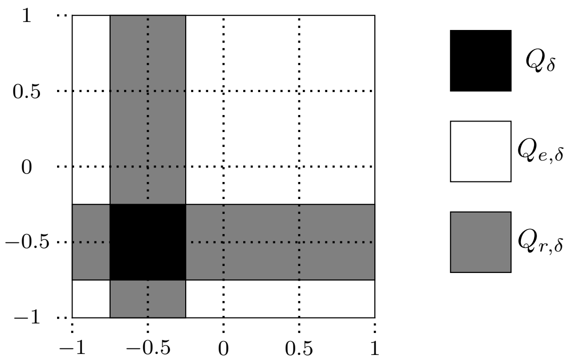

Fig. 4. The different regions of integration for $a = b$ and $\delta = 0.5$.

Having established these two lemmas we proceed with the proof of Theorem 6:

Proof. (Of Theorem 6, Eq. (104) and Eq. (105)). Consider the open interval

$$I := \left(\frac{a}{2} - b, \frac{a}{2} + b\right). \tag{180}$$

If $0 \in I$ (i.e., $|a| < 2b$), set $m := 1 - |a|/(2b)$. If $0 \notin \overline{I}$, set $m := |a|/(2b) - 1$. For $1 > \delta > 0$ we will split the region of integration into several sets, namely the following.

– The bulk contribution:

$$Q_\delta := \left\{(x, y) \in [-1, 1] \times [-1, 1] \,\middle|\, \left|x + \frac{a}{2b}\right|, \left|y + \frac{a}{2b}\right| \leq \delta m\right\}. \tag{181}$$

If $|a| > 2b$, then $Q_\delta := \emptyset$ for every $0 < \delta < 1$.

– The edge contribution:

$$Q_{e,\delta} := \left\{(x, y) \in [-1, 1] \times [-1, 1] \,\middle|\, \left|x + \frac{a}{2b}\right|, \left|y + \frac{a}{2b}\right| > \delta m\right\}. \tag{182}$$

If $|a| > 2b$, then $Q_\delta = [-1, 1] \times [-1, 1]$

– The remaining contribution:

$$Q_{r,\delta} := [-1, 1] \times [-1, 1] \setminus (Q_\delta \cup Q_{e,\delta}). \tag{183}$$

The various regions of integration are depicted in Fig. 4. We will prove the theorem in several steps:

Step 1: *The $Q_{e,\delta}$ contribution of I_1 and I_2 decays exponentially fast*. Formally, we will show that for any $0 < \delta < 1$ and every $\kappa < 2\delta b m \min\{\alpha, 1\}$

$$\lim_{\beta\to\infty} \exp(\kappa\beta) \int\int_{Q_{e,\delta}} dxdy f_{\beta,11}(x, y) \left(f_{\beta,12}(x, y) \pm f_{\beta,13}(x, y)\right) = 0, \tag{184}$$

where we used the same notation as in Eq. (166) (note that this proves Eq. (105)). First of all observe that

$$f_{\beta,11} \left(f_{\beta,12} \pm f_{\beta,13}\right) = |f_{\beta,11}| \cdot |f_{\beta,12} \pm f_{\beta,13}|. \tag{185}$$

Consider the factor $|f_{\beta,11}|$ first. If $x, y > -a/2b + \delta$ or $x, y < -a/2b - \delta$ (this is actually true for all x, y whenever $|a| > 2b$) the mean value theorem yields

$$\begin{aligned} |f_{\beta,11}| &= \beta b \cdot \operatorname{sech}^2\left(\tilde{\epsilon}_\beta(z)\right) \cdot s'_\alpha\left(\tanh\left(\tilde{\epsilon}_\beta(z)\right)\right) \\ &\lesssim (\beta b)^2 C_1 \exp(-2\min\{\alpha, 1\}\, \beta b \delta m). \end{aligned} \tag{186}$$

Here z lies between x and y and C_1 is some constant (any $C_1 > 4\alpha/\log(2)$ works). Here and in the future, we will use the symbol $\lesssim$ to indicate that $\leq$ holds for sufficiently large β.

If $|a| < 2b$ then $x + a/(2b) < -\delta, y + a/(2b) > \delta$ has to be estimated separately. In this case consider the estimate

$$|f_{\beta,11}| \leq \frac{2\sup\{s_\alpha(z)\,||z| \geq \tanh(\delta\beta b m)\}}{2\delta} \lesssim C_{2,\delta,\alpha}\beta b \exp(-2\beta m \delta b \alpha), \tag{187}$$

for some (possibly $\delta-$ and $\alpha-$ dependent) constant $C_{2,\delta,\alpha}$ (the factor βb is actually only needed if $\alpha = 1$). So asymptotically, we have that

$$|f_{\beta,11}| \lesssim (C_1 + C_{2,\delta,\alpha})(b\beta)^2 \exp(-2\min\{\alpha, 1\}\, \beta b \delta m). \tag{188}$$

Consequently, setting $C_2 := C_1 + C_{2,\delta,\alpha}$, we obtain

$$\begin{aligned} &\int_{Q_{e,\delta}} dxdy f_{\beta,11}(x,y)(f_{\beta,12}(x,y) + f_{\beta,13}(x,y)) \\ &\leq C_2(b\beta)^2 \exp(-2\beta b\delta m \min\{\alpha, 1\})J, \end{aligned} \tag{189}$$

where

$$J = \int_{[-1,1]\times[-1,1]} dxdy\, |f_{\beta,12}(x,y)| + |f_{\beta,13}(x,y)|\,. \tag{190}$$

The generalized mean value theorem and some calculus yields

$$\left|\frac{\operatorname{sech}^2(\tilde{\epsilon}_\beta(x)) - \operatorname{sech}^2(\tilde{\epsilon}_\beta(y))}{\tanh(\tilde{\epsilon}_\beta(x)) - \tanh(\tilde{\epsilon}_\beta(x))}\right| \leq 2 \tag{191}$$

and

$$\left|\frac{\operatorname{sech}^2(\tilde{\epsilon}_\beta(x))(1-x^2) - \operatorname{sech}^2(\tilde{\epsilon}_\beta(y))(1-y^2)}{\tanh(\tilde{\epsilon}_\beta(x)) - \tanh(\tilde{\epsilon}_\beta(x))}\right| \leq 2 + \frac{2}{b\beta}. \tag{192}$$

Hence

$$J \lesssim (2+\epsilon)\pi^2 \tag{193}$$

for any $\epsilon > 0$. This together with Eq. (189) yields the identity Eq. (184) and finishes the first step.

Step 2: *The $Q_{r,\delta}$ contribution of I_1 and I_2 is bounded*. Formally we will show that

$$\limsup_{\beta\to\infty} \beta b \int\int_{Q_{r,\delta}} dxdy f_{\beta,11}(x,y)\left(f_{\beta,12}(x,y) \pm f_{\beta,13}(x,y)\right) < \infty. \tag{194}$$

Without any loss of generality we can assume that $\delta < 1/4$. We will will split $Q_{r,\delta}$ into the sets

$$Q_{r,\delta,1} := Q_{r,\delta} \cap \{(x,y) \in [-1,1]\times[-1,1]\,||x-y| < \delta\} \tag{195}$$

and

$$Q_{r,\delta,2} := Q_{r,\delta,1} \setminus Q_{r,\delta,1}. \tag{196}$$

We will show separately that the two integrals

$$J_1 := \beta b \int\int_{Q_{r,\delta,1}} dxdy \, |f_{\beta,11}(x,y)| \left(|f_{\beta,12}(x,y)| + |f_{\beta,13}(x,y)| \right), \tag{197}$$

and

$$J_2 := \beta b \int\int_{Q_{r,\delta,2}} dxdy \, |f_{\beta,11}(x,y)| \left(|f_{\beta,12}(x,y)| + |f_{\beta,13}(x,y)| \right) \tag{198}$$

are bounded. In order to bound J_1, note that by the mean value theorem

$$(|f_{\beta,12}(x,y)| + |f_{\beta,13}(x,y)|) \leq \left(\left(2 + \frac{2}{\beta b} \right) \frac{1}{(1-4\delta^2)^{1/2}(1-\delta^2)^{1/2}} + 2 \right). \tag{199}$$

Hence,

$$J_2 \leq C_\delta \beta b \int\int_{Q_{r,\delta,1}} dxdy \, |f_{11}(x,y)| . \tag{200}$$

An appropriate linear substitution gives

$$\beta b \int\int_{Q_{r,\delta,1}} dxdy \, |f_{11}(x,y)| \tag{201}$$

$$= 2 \int_{\delta b \beta}^{2\delta b \beta} \int_0^{\delta \beta b} dxdy \left| \frac{s_\alpha(\tanh{(x)}) - s_\alpha(\tanh{(y)})}{x-y} \right| . \tag{202}$$

Note that the function $f_\alpha : [0,\infty) \to \mathbb{R}$ defined as $f_\alpha(x) := s_\alpha(\tanh(x))$ is monotoneous decreasing. Moreover,

$$-f_\alpha'(x) = \tag{203}$$

$$\frac{2\alpha}{|1-\alpha|\log(2)} \exp\left(-2\min\{1,\alpha\}\, x\right) \frac{1-\exp(-2\,|\alpha-1|\, x)}{1+\exp(-2\alpha x)} \frac{1}{1+\exp(-2x)}$$

for $\alpha \neq 1$ and

$$-\, f_1'(x) = \frac{4}{\log(2)} \frac{x \exp\left(-2x\right)}{\left(1+\exp(-2x)\right)^2}. \tag{204}$$

Therefore, there exist constants $C_\alpha, \kappa_\alpha > 0$ such that

$$-\, f_\alpha'(x) \leq C_\alpha \exp(-\kappa_\alpha x). \tag{205}$$

That is to say, Lemma 12 gives

$$0 \leq \frac{s_\alpha(\tanh{(x)}) - s_\alpha(\tanh{(y)})}{y-x} \leq \frac{C_\alpha}{\kappa_\alpha} \frac{\exp(-\kappa_\alpha x) - \exp(-\kappa_\alpha y)}{y-x}, \tag{206}$$

giving rise to the estimate

$$\int_{\delta b \beta}^{2\delta b \beta} \int_0^{\delta \beta b} dxdy \left| \frac{s_\alpha(\tanh{(x)}) - s_\alpha(\tanh{(y)})}{x-y} \right| \tag{207}$$

$$\leq \frac{C_\alpha}{(\kappa_\alpha)^2} A_{\delta b \beta \kappa_\alpha, 2\delta b \beta \kappa_\alpha, 0, \delta b \beta \kappa_\alpha},$$

where A_{a_1,a_2,b_1,b_2} has been defined in Lemma 13. By some calculus again

$$\lim_{\beta\to\infty} A_{\delta b\beta\kappa_\alpha,2\delta b\beta\kappa_\alpha,0,\delta b\beta\kappa_\alpha} = \log(2)\,. \tag{208}$$

Therefore, $\limsup_{\beta\to\infty} J_1 < \infty$. In order to bound J_2, the singularities of f_{13} on the lines $x = 1$ and $y = 1$ have to be controlled. We use the bound

$$|f_{1,2}(x,y) + f_{1,3}| \leq \left(4 + \frac{2}{b\beta}\right) \frac{1}{(1-x^2)^{1/2}(1-y^2)^{1/2}} \tag{209}$$

again and bound $f_{1,1}$ in the following way:

$$|f_{1,1}(x,y)| \leq \frac{s_\alpha(\tanh(\tilde{\epsilon}_\beta(x))) + s_\alpha(\tanh(\tilde{\epsilon}_\beta(y))}{\delta}. \tag{210}$$

A short calculation shows that

$$J_2 \lesssim 8\frac{4+\frac{2}{\beta b}}{\delta}(\beta b)^2 C_\alpha \int_0^1 \int_0^1 x \exp(-2\beta\alpha b x)\left(\frac{1}{(1-x^2)^{1/2}(1-y^2)^{1/2}}\right), \tag{211}$$

where C_α is some constant with $C_\alpha > 4\alpha/\log(2)$. Note that

$$\limsup_{\beta\to\infty} \beta^2 \int_0^1 \int_0^1 dxdyx \exp(-2\beta b\alpha x)\frac{1}{(1-x^2)^{1/2}}\frac{1}{(1-y^2)^{1/2}} \leq \frac{\pi}{2(2\alpha b)^2}. \tag{212}$$

This follows easily from explicit integration of the $y-$ integral, giving

$$\int_0^1 dy \frac{1}{(1-y^2)^{1/2}} = \frac{\pi}{2} \tag{213}$$

and an appropriate estimate for the $x-$ integral, namely for fixed $\epsilon > 0$ note that

$$\begin{aligned}
&\int_0^1 dxx \exp(-2\beta b\alpha x)\frac{1}{(1-x^2)^{1/2}} \qquad (214)\\
&\leq \frac{1}{(1-\epsilon^2)^{1/2}} \int_0^\epsilon dxx \exp(-2\beta b\alpha x) + \exp(-2\beta b\alpha\epsilon)\int_\epsilon^1 \frac{1}{(1-x^2)^{1/2}}\\
&\leq \frac{1}{(2\alpha b\beta)^2(1-\epsilon^2)^{1/2}} + \exp(-\epsilon\beta b)\frac{\pi}{2}.
\end{aligned}$$

Finally, multiply this expression by β^2, take the $\limsup$ for β to infinity and let ϵ approach zero afterwards (bounding $1/(1-x^2)^{1/2}$ by 1 from below actually shows that Eq. (212) holds true with equality and that the limit superior is actually a limit). In any case J_2 is bounded, proving the second step.

Step 3: *The integrand $f_{\beta,11}$ bounds the asymptotic growth of I_1 and I_2*. Formally we will show that

$$\limsup_{\beta\to\infty} \frac{I_1}{\log(\beta)} \leq \liminf_{\beta\to\infty} \frac{4\beta b \int_{Q_\delta} dxdy\,|f_{\beta,11}(x,y)|}{\log(\beta)} \tag{215}$$

and

$$\limsup_{\beta\to\infty} \frac{I_2}{\log(\beta)} \leq \liminf_{\beta\to\infty} \frac{4\beta b \int_{Q_\delta} dxdy\, |f_{\beta,11}(x,y)|}{\log(\beta)} \tag{216}$$

for any $0 < \delta < 1$. The result for I_2 is trivial when the result for I_1 is settled, since $I_2 \leq I_1$. Fix $\epsilon > 0$ and note that by Step 1 and Step 2, we find that

$$\limsup_{\beta\to\infty} \frac{I_1}{\log(\beta)} = \limsup_{\beta\to\infty} \frac{I_{1,\epsilon}}{\log(\beta)} \tag{217}$$

where

$$I_{1,\epsilon} := b\beta \int\int_{Q_\epsilon} dxdy f_{11}(x,y) \left(f_{12}(x,y) + f_{13}(x,y)\right). \tag{218}$$

However, for $x, y \in Q_\epsilon$ the mean value theorem yields the estimate

$$|f_{12}(x,y) + f_{13}(x,y)| \leq 2 + 2\left(1 + \frac{1}{\beta b}\right)\frac{1}{1-\epsilon^2} \tag{219}$$

again (compare Step 1 and Step 2). This is especially true for the choice $0 < \epsilon < \delta$, and therefore

$$\begin{aligned}\limsup_{\beta\to\infty} \frac{I_1}{\log(\beta)} &\leq \liminf_{\beta\to\infty}\left(2 + 2\frac{1}{1-\epsilon^2}\right)\frac{\beta b \int_{Q_\epsilon} dxdy\, |f_{\beta,11}(x,y)|}{\log(\beta)} \\ &\leq \liminf_{\beta\to\infty}\left(2 + 2\frac{1}{1-\epsilon^2}\right)\frac{\beta b \int_{Q_\delta} dxdy\, |f_{\beta,11}(x,y)|}{\log(\beta)}. \end{aligned}\tag{220}$$

In the last expression ϵ can be sent to zero, proving the upper bound, Eq. (215).

Step 4: *Derive a logarithmic bound for I_1 and show that I_2 increases sub-logarithmically.* We will show that

$$\limsup_{\beta\to\infty} \frac{I_1}{\log(\beta)} \leq \min\left\{\frac{108\alpha}{\log(2)\min\{1,\alpha\}^3}, \frac{16\alpha}{\log(2)\,|1-\alpha|\min\{1,\alpha\}^2}\right\} \tag{221}$$

and

$$\limsup_{\beta\to\infty} \frac{I_2}{\log(\beta)} = 0. \tag{222}$$

We use Eq. (215) from Step 3, with which we make a linear substitution and exploit the symmetry of the integrand to get

$$\limsup_{\beta\to\infty} \frac{I_1}{\log(\beta)} \leq \limsup_{\beta\to\infty} \frac{8\left(J_{11} + J_{12}\right)}{\log(\beta)}, \tag{223}$$

where

$$J_{11} = \int_0^{\delta\beta b}\int_0^{\delta\beta b} dxdy \frac{f_\alpha(x) - f_\alpha(y)}{y - x} \tag{224}$$

and

$$J_{12} = \int_0^{\delta\beta b}\int_0^{\delta\beta b} dxdy \frac{f_\alpha(x) + f_\alpha(y)}{x + y}. \tag{225}$$

Here, f_α are the functions introduced in Step 2. Fix $0 < \epsilon < \min\{\alpha, 1\}$. By Eq. (205), one finds

$$-{f_\alpha}'(x) \leq C_\alpha \exp(-\kappa_\alpha x). \tag{226}$$

A look at Eq. (205) and Eq. (204) in turn reveals that

$$C_\alpha := \frac{2\alpha}{\log(2)\epsilon}, \kappa_\alpha := 2(\min\{\alpha, 1\} - \epsilon) \tag{227}$$

is a possible choice. Proceeding as in Step 3 yields

$$\limsup_{\beta\to\infty} \frac{J_{11}}{\log(\beta)} \leq \limsup_{\beta\to\infty} \frac{C_\alpha}{(\kappa_\alpha)^2} \frac{A_{0,\delta b\beta\kappa_\alpha,0,\delta b\beta\kappa_\alpha}}{\log(\beta)} = \frac{2C_\alpha}{(\kappa_\alpha)^2} \tag{228}$$

and optimizing for ϵ gives

$$\limsup_{\beta\to\infty} \frac{J_{11}}{\log(\beta)} \leq \frac{27\alpha}{8\log(2)\left(\min\{1, \alpha\}\right)^3}. \tag{229}$$

Another possibility (working for $\alpha \neq 1$ only) is to use the bound

$$-{f_\alpha}'(x) \leq \frac{2\alpha}{|1-\alpha|\log(2)} \exp(-2\min\{a, 1\}\, x), \tag{230}$$

giving the asymptotic bound

$$\limsup_{\beta\to\infty} \frac{J_{11}}{\log(\beta)} \leq \frac{\alpha}{|1-\alpha|\log(2)\left(\min\{a, 1\}\right)^2}. \tag{231}$$

To bound J_{12}, note that $x + y \geq |x - y|$ for any $x, y \geq 0$. Therefore,

$$J_{12} \leq J_{11}. \tag{232}$$

To show the validity of Eq. (222), we use the mean value theorem to yield the following bounds

$$\left| \frac{\operatorname{sech}^2(\tilde\epsilon_\beta(x)) - \operatorname{sech}^2(\tilde\epsilon_\beta(y))}{\tanh(\tilde\epsilon_\beta(x)) - \tanh(\tilde\epsilon_\beta(x))} \left(\frac{1}{\sqrt{1-x^2}\sqrt{1-y^2}} - 1 \right) \right| \leq 2\left(\frac{1}{1-\delta^2} - 1 \right) \tag{233}$$

for all $x, y \in Q_\delta$. By the same argument,

$$\left| \frac{x^2\operatorname{sech}^2(\tilde\epsilon_\beta(x)) - y^2\operatorname{sech}^2(\tilde\epsilon_\beta(y))}{\tanh(\tilde\epsilon_\beta(x)) - \tanh(\tilde\epsilon_\beta(x))} \left(\frac{1}{\sqrt{1-x^2}\sqrt{1-y^2}} \right) \right| \leq \frac{\frac{2\delta}{\beta b} + 2\delta^2}{1-\delta^2} \tag{234}$$

and therefore

$$|f_{12} - f_{13}| \leq 2\left(\frac{2\delta^2 + \frac{\delta}{\beta b}}{1-\delta^2} \right), \tag{235}$$

repeating the argument for the I_1 integral yields the existence of some constant $C_\alpha > 0$ such that

$$\limsup_{\beta\to\infty} \frac{I_1}{\log(\beta)} \leq C_\alpha 2\left(\frac{2\delta^2}{1-\delta^2} \right). \tag{236}$$

Since this is true for all $\delta \geq 0$, we have

$$\limsup_{\beta\to\infty} \frac{I_1}{\log(\beta)} = 0, \tag{237}$$

finishing Step 4.

Therefore for $|a| < 2b$, by Step 4 and Eq. (161),

$$\begin{aligned} \limsup_{\beta\to\infty} \frac{I_{\alpha,\infty}(A:B)}{\log(\beta)} &\leq \limsup_{\beta\to\infty} \frac{2J_{11}}{\pi^2 \log(\beta)} \qquad (238) \\ &\leq \frac{2\alpha}{\pi^2 \log(2) \left(\min\{1,\alpha\}\right)^2} \min\left\{ \frac{27}{2\left(\min\{1,\alpha\}\right)}, \frac{4}{|1-\alpha|} \right\}, \end{aligned}$$

completing the proof of the low-temperature limit. $\square$